

STIC Search Report

EIC 1700

STIC Database Tracking Number: 174792

**TO: Rabon A Sergeant
Location: REM 10D65
Art Unit : 1711
December 28, 2005**

Case Serial Number: 09/485533

**From: Usha Shrestha
Location: EIC 1700
REMSEN 4B28
Phone: 571/272-3519
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Search Notes

=> fil reg

FILE 'REGISTRY' ENTERED AT 13:15:17 ON 28 DEC 2005

=> d his

FILE 'HCAPLUS' ENTERED AT 08:17:15 ON 28 DEC 2005

L1 1 S WO1998-FR01800/PRN,AP
SEL RN

FILE 'REGISTRY' ENTERED AT 08:18:23 ON 28 DEC 2005

L2 12 S E1-E12
L3 889 S 4.264.1/RID
L4 15227 S 46.492.1/RID
E URETDIONE
E URETIDINEDIONE/CN
E URETIDIONE/CN
E URETDIONE/CN
L5 1 S E10
L6 71218 S PUR/PCT
L7 2 S L2 AND L6
L8 162 S L3 AND L6
L9 7609 S L6 NOT 1-50/NR
L10 1 S 220652-25-5/RN
L11 1 S 220588-31-8/RN
L12 245445 S OTHER/PCT
L13 81225 S OTHERO/PCT
L14 245445 S L12 OR L13
L15 2 S L14 AND L2
L16 68 S L14 AND L3
L17 98094 S L14 NOT 2-100/NR
L18 8 S L17 AND L3
L19 4617 S PIR/PCT
L20 0 S L19 AND L2
L21 339 S L19 NOT 1-100/NR
L22 154 S L3 NOT 2-100/NR
L23 42 S L19 AND L3
L24 1 S L23 NOT 2-100/NR
L25 10 S L8 NOT 2-100/NR

FILE 'HCAPLUS' ENTERED AT 12:10:19 ON 28 DEC 2005

L26 734 S L3
L27 5 S L18
L28 1 S L24
L29 5 S L25
L30 9 S L27-L29
L31 323 S L26 (L) PREP/RL
L32 82 S L31 (L) (?URETHAN? OR ?ISOCYANAT?)
L33 32 S L32 AND (HEAT? OR TEMP?)
L34 12 S L33 NOT CAT?
L35 242 S L31 NOT CAT?
L36 68 S L35 AND (HEAT? OR TEMP?)
L37 24 S L32 AND CAT/RL
L38 58 S L32 NOT L37
L39 17 S L38 AND (HEAT? OR TEMP?)

FILE 'REGISTRY' ENTERED AT 12:30:34 ON 28 DEC 2005

L40 154 S L3 NOT 2-100/NR

FILE 'HCAPLUS' ENTERED AT 12:31:05 ON 28 DEC 2005

L41 180 S L40

L42 77 S L41(L) PREP/RL
L43 27 S L42(L) (?URETHAN? OR ?ISOCYANAT?)
L44 54 S L42 AND (?URETHAN? OR ?ISOCYANAT?)
L45 13 S L44 AND CAT?/RL
L46 41 S L44 NOT L45
L47 18 S L46 AND (HEAT? OR TEMP?)
L48 1 S L47 AND L1
L49 27 S L30 OR L47
L50 46 S L46 OR L47 OR L49

=> d que 150

L3 889 SEA FILE=REGISTRY ABB=ON PLU=ON 4.264.1/RID
L6 71218 SEA FILE=REGISTRY ABB=ON PLU=ON PUR/PCT
L8 162 SEA FILE=REGISTRY ABB=ON PLU=ON L3 AND L6
L12 245445 SEA FILE=REGISTRY ABB=ON PLU=ON OTHER/PCT
L13 81225 SEA FILE=REGISTRY ABB=ON PLU=ON OTHERO/PCT
L14 245445 SEA FILE=REGISTRY ABB=ON PLU=ON L12 OR L13
L17 98094 SEA FILE=REGISTRY ABB=ON PLU=ON L14 NOT 2-100/NR
L18 8 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND L3
L19 4617 SEA FILE=REGISTRY ABB=ON PLU=ON PIR/PCT
L23 42 SEA FILE=REGISTRY ABB=ON PLU=ON L19 AND L3
L24 1 SEA FILE=REGISTRY ABB=ON PLU=ON L23 NOT 2-100/NR
L25 10 SEA FILE=REGISTRY ABB=ON PLU=ON L8 NOT 2-100/NR
L27 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L18
L28 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L24
L29 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L25
L30 9 SEA FILE=HCAPLUS ABB=ON PLU=ON (L27 OR L28 OR L29)
L40 154 SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT 2-100/NR
L41 180 SEA FILE=HCAPLUS ABB=ON PLU=ON L40
L42 77 SEA FILE=HCAPLUS ABB=ON PLU=ON L41(L) PREP/RL
L44 54 SEA FILE=HCAPLUS ABB=ON PLU=ON L42 AND (?URETHAN? OR
?ISOCYANAT?)
L45 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L44 AND CAT?/RL
L46 41 SEA FILE=HCAPLUS ABB=ON PLU=ON L44 NOT L45
L47 18 SEA FILE=HCAPLUS ABB=ON PLU=ON L46 AND (HEAT? OR
TEMP?)
L49 27 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 OR L47
L50 46 SEA FILE=HCAPLUS ABB=ON PLU=ON L46 OR L47 OR L49

=> fil hcap

FILE 'HCAPLUS' ENTERED AT 13:15:35 ON 28 DEC 2005

=> => d 150 1-46 ibib abs hitstr hitind

L50 ANSWER 1 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:405056 HCAPLUS

DOCUMENT NUMBER: 142:433133

TITLE: Urethonimines bearing double bonds, their
polymers, gels, ion-conductive compositions,
and their applications

INVENTOR(S): Aizawa, Wakana; Iida, Kazuyuki

PATENT ASSIGNEE(S): Mitsubishi Paper Mills, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.

CODEN: JKXXAF

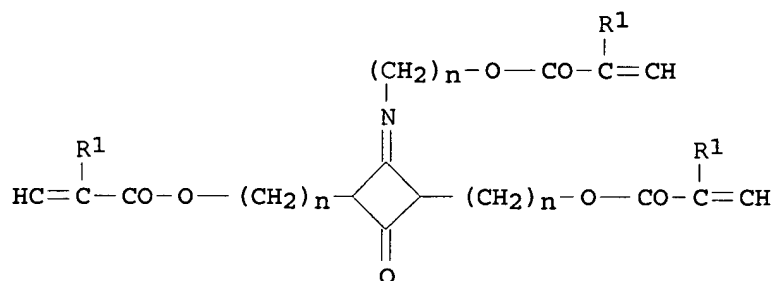
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005119969	A2	20050512	JP 2003-353147	2003 1014
PRIORITY APPLN. INFO.:				2003 1014
				2003 1014

OTHER SOURCE(S): MARPAT 142:433133
GI



AB The urethonimines are I (R¹ = H, alkyl; n = 2-6). The urethonimines are polymerized in various solvents without undesired side reactions between carbodiimide groups and active H. The polymers, useful as electrolytes for electrochem. devices, e.g., secondary Li batteries, capacitors, and surface modifiers, show good heat resistance because they generate isocyanate and carbodimide groups suppressing hydrolysis.

IT 850789-28-5P 850789-29-6P 850789-30-9P
850789-32-1P

(urethonimines bearing double bonds for ion-conductive polymer gels showing good heat resistance for secondary Li batteries, double-layer capacitors, and surface modifiers)

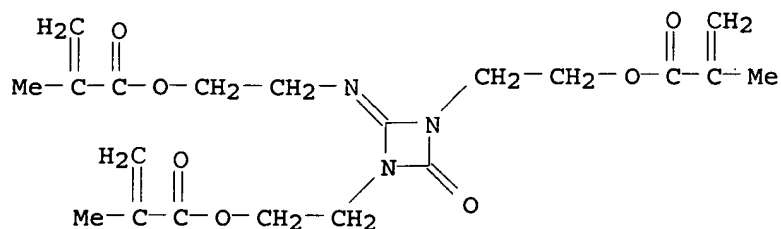
RN 850789-28-5 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, methanetetraylbis(nitrilo-2,1-ethanediyl) ester, polymer with [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidene-1,3-diyl]di-2,1-ethanediyl bis(2-methyl-2-propenoate) (9CI) (CA INDEX NAME)

CM 1

CRN 850789-27-4

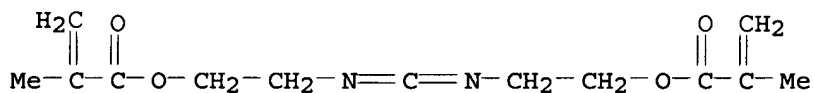
CMF C20 H27 N3 O7



CM 2

CRN 817619-67-3

CMF .C13 H18 N2 O4



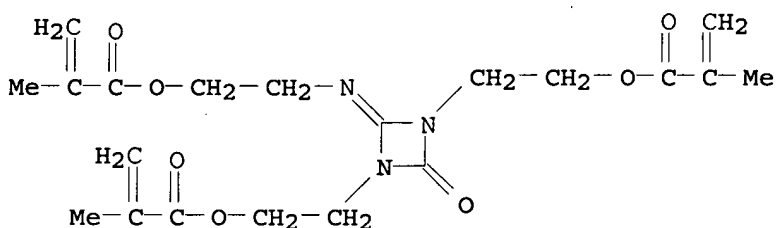
RN 850789-29-6 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidino-1,3-diyl]di-2,1-ethanediyl ester, polymer with α -(2-methyl-1-oxo-2-propenyl)- ω -methoxypoly(oxy-1,2-ethanediyl) (9CI) (CA INDEX NAME)

CM 1

CRN 850789-27-4

CMF C20 H27 N3 O7

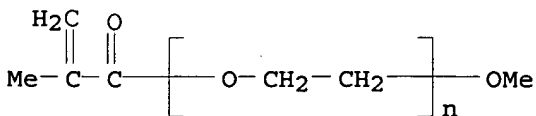


CM 2

CRN 26915-72-0

$$\text{CMF} \quad (\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_5 \text{ H}_8 \text{ O}_2$$

CCI PMS



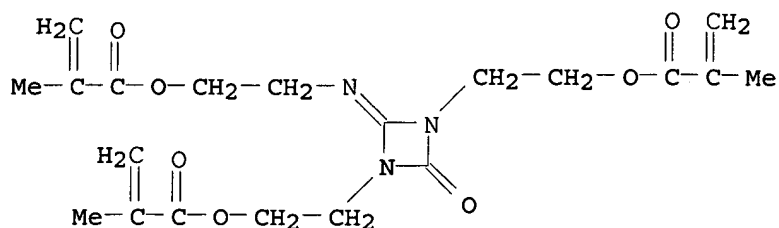
RN 850789-30-9 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidine-1,3-diyl]di-2,1-ethanediyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 850789-27-4

CMF C20 H27 N3 O7



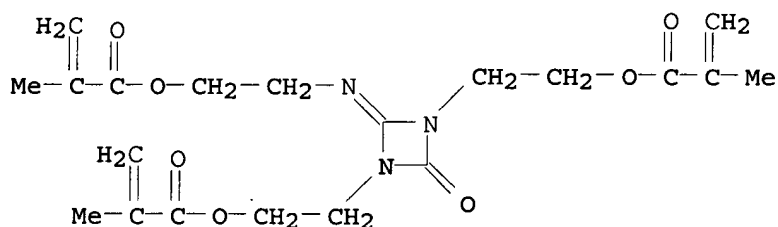
RN 850789-32-1 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidine-1,3-diyl]di-2,1-ethanediyl ester, polymer with ethene, graft (9CI) (CA INDEX NAME)

CM 1

CRN 850789-27-4

CMF C20 H27 N3 O7



CM 2

CRN 74-85-1

CMF C2 H4

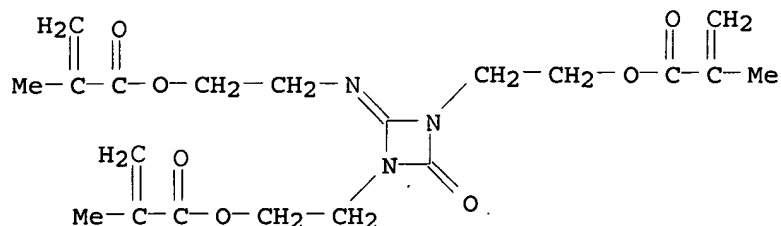
H₂C=CH₂

IT 850789-27-4P

(urethonimines bearing double bonds for ion-conductive polymer gels showing good heat resistance for secondary Li batteries, double-layer capacitors, and surface modifiers)

RN 850789-27-4 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidinediyl]di-2,1-ethanediyl ester (9CI) (CA INDEX NAME)



IT 850789-31-0P

(urethonimines bearing double bonds for ion-conductive polymer gels showing good heat resistance for secondary Li batteries, double-layer capacitors, and surface modifiers)

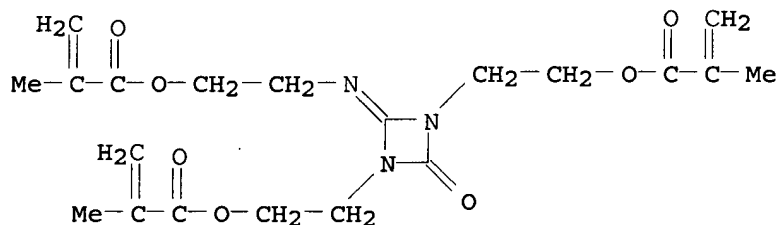
RN 850789-31-0 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, methanetetraylbis(nitrilo-2,1-ethanediyl) ester, polymer with [2-[[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]imino]-4-oxo-1,3-diazetidino-1,3-diyl]di-2,1-ethanediyl bis(2-methyl-2-propenoate) and α -(1-oxo-2-propenyl)- ω -methoxypoly(oxy-1,2-ethanediyl) (9CI). (CA INDEX NAME)

CM 1

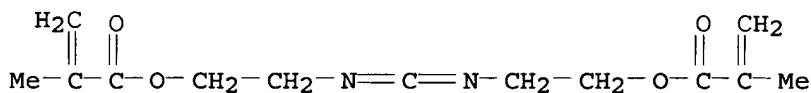
CRN 850789-27-4

CMF C20 H27 N3 O7



CM 2

CRN 817619-67-3

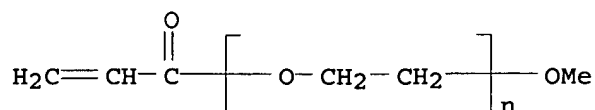
CMF C13 H18 N2 O4

CM 3

CRN 32171-39-4

$$\text{CMF} \quad (\text{C}_2 \text{ H}_4 \text{ O})_n \text{ C}_4 \text{ H}_6 \text{ O}_2$$

CCI PMS



- IC ICM C07D229-00
ICS C08F020-36; C08F291-00; C08F292-00; H01G009-038; H01M010-40
- CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 28, 35, 38, 76
- ST urethonimine polymer ionic conductor **heat** resistance;
lithium battery urethonimine polymer gel electrolyte; capacitor
urethonimine polymer gel electrolyte; surface modifier
urethonimine polymer
- IT Polyoxyalkylenes, uses
(acrylic, urethonimine-containing; urethonimines bearing double
bonds for ion-conductive polymer gels showing good **heat**
resistance for secondary Li batteries, double-layer capacitors,
and surface modifiers)
- IT Capacitors
(double layer; urethonimines bearing double bonds for
ion-conductive polymer gels showing good **heat**
resistance for secondary Li batteries, double-layer capacitors,
and surface modifiers)
- IT Secondary batteries
(lithium; urethonimines bearing double bonds for ion-conductive
polymer gels showing good **heat** resistance for
secondary Li batteries, double-layer capacitors, and surface
modifiers)
- IT Surface treatment
(modifiers; urethonimines bearing double bonds for
ion-conductive polymer gels showing good **heat**
resistance for secondary Li batteries, double-layer capacitors,
and surface modifiers)
- IT Ionic conductors
(polymeric; urethonimines bearing double bonds for
ion-conductive polymer gels showing good **heat**
resistance for secondary Li batteries, double-layer capacitors,
and surface modifiers)
- IT Electrolytic capacitors
Gels
Heat-resistant materials
Polymer electrolytes
(urethonimines bearing double bonds for ion-conductive polymer
gels showing good **heat** resistance for secondary Li
batteries, double-layer capacitors, and surface modifiers)
- IT 850789-28-5P 850789-29-6P 850789-30-9P
850789-32-1P
(urethonimines bearing double bonds for ion-conductive polymer
gels showing good **heat** resistance for secondary Li
batteries, double-layer capacitors, and surface modifiers)
- IT 817619-67-3P 850789-27-4P
(urethonimines bearing double bonds for ion-conductive polymer
gels showing good **heat** resistance for secondary Li
batteries, double-layer capacitors, and surface modifiers)
- IT 850789-31-0P
(urethonimines bearing double bonds for ion-conductive polymer
gels showing good **heat** resistance for secondary Li
batteries, double-layer capacitors, and surface modifiers)
- IT 30674-80-7

(urethonimines bearing double bonds for ion-conductive polymer gels showing good heat resistance for secondary Li batteries, double-layer capacitors, and surface modifiers)

L50 ANSWER 2 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:20011 HCAPLUS

DOCUMENT NUMBER: 140:78231

TITLE: Pressure-sensitive acrylic adhesives without foaming nor substrate staining and polarizing films therewith showing good processability

INVENTOR(S): Ebata, Norimitsu; Miyazaki, Hideki; Nakagawa, Nobuo; Uemae, Masami

PATENT ASSIGNEE(S): Nippon Carbide Industries Co., Inc., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2004002782	A2	20040108	JP 2003-98425	2003 0401
PRIORITY APPLN. INFO.:			JP 2002-103154	A 2002 0405

AB The adhesives comprise (A) high-mol.-weight acrylic copolymers [Mw 900,000-2,500,000, Tg \leq -45°, SP 8.7-9.3 (SP = solubility parameter)] having reactive functional groups 100, (B) low-mol.-weight acrylic copolymers (Mw 50,000-200,000, Tg -40 to 0°, SP 8.7-9.3) prepared from (b1) H₂C:CHCO₂R₁ [R₁ = C₄-10 (branched) alkyl] whose homopolymers satisfy Tg \leq -50°, (b2) monomers relatively less copolymerizable with b1, and (b3) monomers relatively highly copolymerizable with b1 5-100, and (C) polyfunctional compds. crosslinkable with A 0.001-10 parts. Thus, acrylic acid-n-Bu acrylate (BA) copolymer (Mw 1,200,000, Tg -55°, SP 9.1) was mixed with BA-n-Bu methacrylate-Me acrylate copolymer (Mw 90,000, Tg -15°, SP 9.1) and Duranate E 405-80T (modified HMDI) to give an adhesive composition, which was applied on a release film, laminated with poly(vinyl alc.)/cellulose triacetate polarizing film, and dried to give adhesive layer-equipped film. The film was bonded on a glass sheet showing 180° peel strength 450 and 700 g/25 mm, after aging at 23° and 70°, resp., no foaming nor light-leaking defect after 1000-h aging at 100°, and no glass staining after peeling.

IT 641636-24-0P

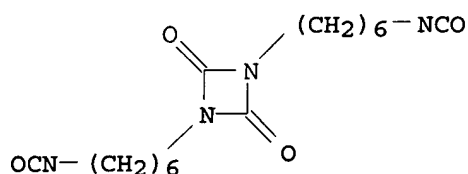
(pressure-sensitive acrylic adhesives without foaming nor substrate staining useful for polarizing films)

RN 641636-24-0 HCAPLUS

CN 2-Propenoic acid, polymer with 1,3-bis(6-isocyanatohexyl)-1,3-diazetidene-2,4-dione and butyl 2-propenoate (9CI) (CA INDEX NAME)

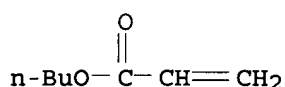
CM 1

CRN 23501-81-7
CMF C16 H24 N4 O4



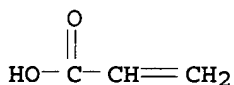
CM 2

CRN 141-32-2
CMF C7 H12 O2



CM 3

CRN 79-10-7
CMF C3 H4 O2



IC ICM C09J133-08
ICS C09J133-02; C09J133-10; C09J163-00; C09J175-04; C09J183-08
CC 38-3 (Plastics Fabrication and Uses)
Section cross-reference(s): 73, 74
IT 77-99-6DP, Trimethylolpropane, reaction products with (hydrogenated) xylylene diisocyanate or HMDI, polymers with acrylic acid copolymers 822-06-0DP, HMDI, modified, polymers with acrylic acid copolymers 25854-16-4DP, Xylylene diisocyanate, reaction products with trimethylolpropane, polymers with acrylic acid-n-Bu acrylate-2-hydroxyethyl acrylate copolymer 42170-25-2DP, reaction products with trimethylolpropane, polymers with acrylic acid-n-Bu acrylate copolymer 152048-77-6P, Acrylic acid-n-butyl acrylate-TETRAD-C copolymer 416844-24-1P 416844-36-5P, Acrylic acid-n-butyl acrylate-Desmodur N 3400 copolymer 556818-60-1P, Acrylic acid-butyl acrylate-Takenate D 120N copolymer 556818-63-4P, Acrylic acid-n-butyl acrylate-Coronate HX copolymer 641620-83-9P, Acrylic acid-n-butyl acrylate-Duranate E 405-80T copolymer 641620-84-0P 641620-85-1P 641620-86-2P 641620-87-3P, Acrylic acid-n-butyl acrylate-Coronate HL-S copolymer 641620-88-4P, Acrylic acid-butyl acrylate-2-ethylhexyl acrylate-methyl acrylate-Takenate M 631N copolymer 641620-89-5P, Acrylic acid-butyl acrylate-ethyl acrylate-Duranate E 405-80T-2-ethylhexyl acrylate copolymer 641620-90-8P, Acrylic

acid-butyl acrylate-Duranate E 405-80T-methyl methacrylate
 copolymer 641636-19-3P, Acrylic acid-n-butyl
 acrylate-hexamethylene diisocyanate isocyanurate
 copolymer 641636-24-0P
 (pressure-sensitive acrylic adhesives without foaming nor
 substrate staining useful for polarizing films)

L50 ANSWER 3 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:359890 HCAPLUS

DOCUMENT NUMBER: 136:355793

TITLE: Diisocyanatononane-based
 polyisocyanates

INVENTOR(S): Suzuki, Shigeaki; Hori, Hiroshi

PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2002138129	A2	20020514	JP 2000-335981	2000 1102
PRIORITY APPLN. INFO.:			JP 2000-335981	2000 1102

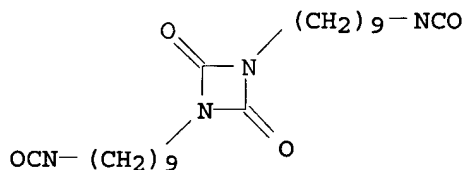
AB The polyisocyanates are manufactured by either of (a) biuret formation of 1,9-diisocyanatononane (I) or 1,8-diisocyanato-2-methyloctane (II), (b) reaction of I or II with polyol, or (c) cyclodimerization of I or II. I and II show low vapor pressure and the polyisocyanates show high reactivity. Thus, I was treated with H₂O in the presence of Me₃PO₄ to give biuret polyisocyanate.

IT 420135-71-3P 420789-42-0P

(manufacture of diisocyanatononane-based
 polyisocyanates)

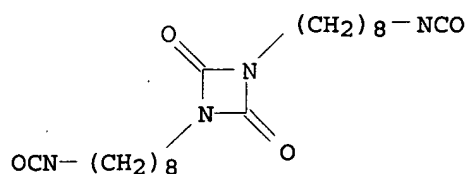
RN 420135-71-3 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(9-isocyanatononyl)- (9CI) (CA INDEX NAME)



RN 420789-42-0 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis[8-isocyanato-2(or 7)-methyloctyl]- (9CI) (CA INDEX NAME)



2 (D1-Me)

IC ICM C08G018-73
ICS C08G018-10
CC 37-2 (Plastics Manufacture and Processing)
ST **isocyanatononane polyisocyanate** manuf; biuret
polyisocyanate diisocyanatononane manuf; polyol
diisocyanatononane adduct polyisocyanate manuf;
cyclodimerization **diisocyanatononane**
polyisocyanate manuf
IT 420135-69-9P 420135-70-2P
(biuret-type, oligomeric; manufacture of **diisocyanatononane**
-based **polyisocyanates**)
IT 77-99-6DP, Trimethylolpropane, reaction products with
diisocyanato(iso)nonane 7192-79-2DP, reaction products
with trimethylolpropane 176506-52-8DP, reaction products with
trimethylolpropane 420135-71-3P 420789-42-0P
(manufacture of **diisocyanatononane**-based
polyisocyanates)
IT 7192-79-2 176506-52-8
(manufacture of **diisocyanatononane**-based
polyisocyanates)

L50 ANSWER 4 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:711613 HCAPLUS

DOCUMENT NUMBER: 136:69773

TITLE: Synthesis of N-functionalized carbodiimides,
hydantoins, 1,3-diazetidines, and
imidazolidine derivatives from N-vinyl
phosphazenes derived from β -amino acids

AUTHOR(S): Palacios, Francisco; Legido, Marta; Perez de
Heredia, Itziar; Ezpeleta, Jose Maria;
Rubiales, Gloria

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de
Farmacia, Universidad del Pais Vasco, Vitoria,
01080, Spain

SOURCE: Heterocycles (2001), 55(9), 1641-1651

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:69773

AB Synthesis of N-vinyl carbodiimides through aza-Wittig reaction
of N-vinyl phosphazenes with **isocyanates** is reported.
These heterocumulenes are used for the preparation of unsym. ureas and
nitrogen heterocycles such as hydantoins, 1,3-diazetidines,
imidazolidinones, and bis-imidazolidinone azines.

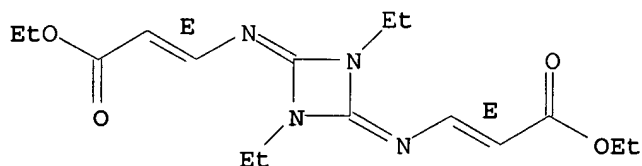
IT 384372-45-6P 384372-46-7P
(preparation of N-functionalized carbodiimides, hydantoins,

1,3-diazetidines, and imidazolidine derivs. from N-vinyllic phosphazenes derived from β -amino acids)

RN 384372-45-6 HCAPLUS

CN 2-Propenoic acid, 3,3'-[(1,3-diethyl-1,3-diazetidine-2,4-diylidene)dinitrilo]bis-, diethyl ester, (2E,2'E)- (9CI) (CA INDEX NAME)

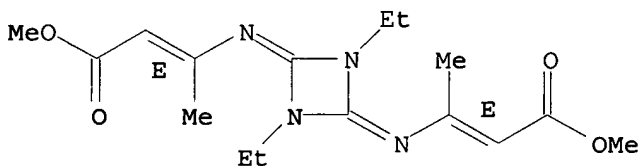
Double bond geometry as shown.



RN 384372-46-7 HCAPLUS

CN 2-Butenoic acid, 3,3'-[(1,3-diethyl-1,3-diazetidine-2,4-diylidene)dinitrilo]bis-, dimethyl ester, (2E,2'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

ST carbodiimide deriv prepn hydration; hydantoin deriv prepn; diazetidine deriv prepn; imidazolidine deriv prepn; phosphazene vinyllic reaction **isocyanate**

IT 103-71-9, Phenyl **isocyanate**, reactions 109-90-0, Ethyl **isocyanate** 110-78-1, Propyl **isocyanate** 81777-30-2 152975-95-6 152975-96-7 384372-48-9 384372-49-0 384372-51-4 421598-34-7

(preparation of N-functionalized carbodiimides, hydantoins, 1,3-diazetidines, and imidazolidine derivs. from N-vinyllic phosphazenes derived from β -amino acids)

IT 384372-39-8P 384372-40-1P 384372-41-2P 384372-42-3P 384372-44-5P 384372-45-6P 384372-46-7P 384372-47-8P 384372-50-3P 384842-74-4P 384842-75-5P 384842-76-6P 384842-77-7P 384842-78-8P

(preparation of N-functionalized carbodiimides, hydantoins, 1,3-diazetidines, and imidazolidine derivs. from N-vinyllic phosphazenes derived from β -amino acids)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 5 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:581955 HCAPLUS

DOCUMENT NUMBER: 135:153862

TITLE: Preparation of two component polyurethane foam compositions for sound and vibration absorbers
INVENTOR(S): Bicknell, Rodney; Kirkham, Helen; Spencer,

PATENT ASSIGNEE(S): Richard
 SOURCE: Baxenden Chemicals Limited, UK
 PCT Int. Appl., 23 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001057107	A1	20010809	WO 2001-GB408	

2001
0131

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1254187	A1	20021106	EP 2001-948990	
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2001
0131

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2003119929	A1	20030626	US 2002-182678	
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2002
0903

PRIORITY APPLN. INFO.:

GB 2000-2175

A

2000
0131

WO 2001-GB408

W

2001
0131

AB The process comprises mixing (A) a polyol resin component, (B) an isocyanate component having a free monomeric diisocyanate content of ≤ 2 wt%, and (C) a catalyst blend comprising ≥ 2 catalytic materials selected from (a) organometallic catalysts, (b) amines, and (c) isocyanurate catalysts. Thus a polyurethane foam was prepared by mixing of polyoxypropylated glycerol, polyoxypropylated toluene diamine, polyoxypropylene diol, diethanolamine, B 8404, triethylene glycol diamine, dibutyltin dilaurate, Baxcat 0, tri(3-dimethylaminopropyl)amine, hexamethylene diisocyanate biuret, and propylene carbonate with tetrafluoroethane, showing core d. 100-120 kg/m³, closed cell content (ASTM D2856) 3.6%, and flammability 3.05 cm/min (1.2 in./min) determined by MVSS-320 test.

IT 353245-35-9P 353245-36-0P

(preparation of two component polyurethane foam compns. for sound and vibration absorbers)

RN 353245-35-9 HCAPLUS

CN 1,3-Diazetidene-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer

with Castomer E 1004, α -hydro- ω -hydroxypoly[oxy(methyl-1,2-ethanediyl)] and α,α',α'' -1,2,3-propanetriyltris[ω -hydroxypoly[oxy(methyl-1,2-ethanediyl)]] (9CI) (CA INDEX NAME)

CM 1

CRN 353244-60-7

CMF Unspecified

CCI PMS, MAN

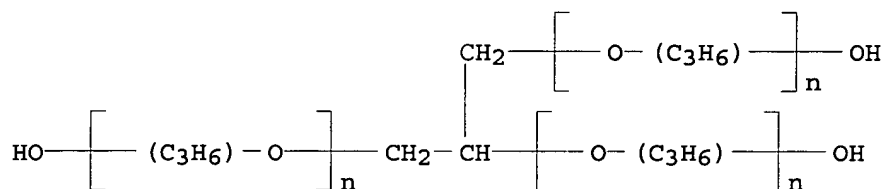
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 25791-96-2

CMF (C3 H6 O)_n (C3 H6 O)_n (C3 H6 O)_n C3 H8 O3

CCI IDS, PMS

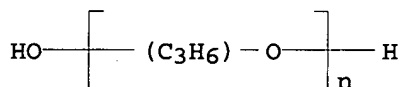


CM 3

CRN 25322-69-4

CMF (C3 H6 O)_n H2 O

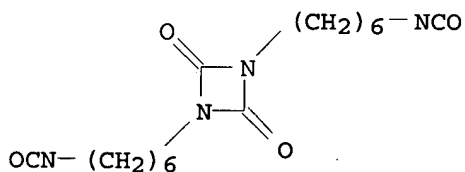
CCI IDS, PMS



CM 4

CRN 23501-81-7

CMF C16 H24 N4 O4



RN 353245-36-0 HCAPLUS

CN 1,3-Diazetidone-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with Castomer E 1004, α -hydro- ω -hydroxypoly(oxy-1,2-

ethanediyl) and $\alpha, \alpha', \alpha''$ -1,2,3-
propanetriyltris[ω -hydroxypoly[oxy(methyl-1,2-ethanediyl)]]
(9CI) (CA INDEX NAME)

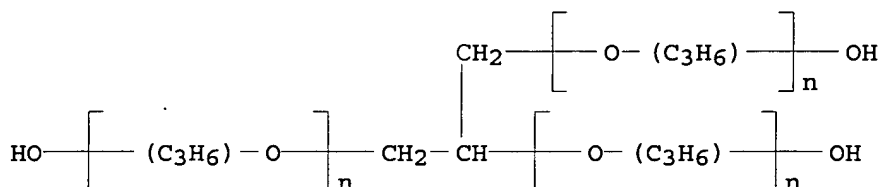
CM 1

CRN 353244-60-7
CMF Unspecified
CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

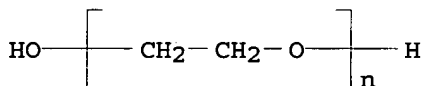
CM 2

CRN 25791-96-2
CMF (C3 H6 O)_n (C3 H6 O)_n (C3 H6 O)_n C3 H8 O3
CCI IDS, PMS



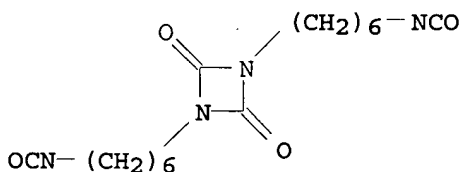
CM 3

CRN 25322-68-3
CMF (C2 H4 O)_n H2 O
CCI PMS



CM 4

CRN 23501-81-7
CMF C16 H24 N4 O4



IC ICM C08G018-16
CC 38-3 (Plastics Fabrication and Uses)
Section cross-reference(s): 29, 67
IT 4035-89-6DP, Hexamethylene diisocyanate biuret, polymers with

Mannich base and polyoxypropylated glycerol 23501-81-7DP,
 polymers with Mannich base, polyoxypropylated glycerol, and TDI
 prepolymer 25791-96-2DP, polymers with Mannich base,
 hexamethylene diisocyanate uretdione, and TDI prepolymer
 26471-62-5DP, TDI, polymers with Mannich base, polyoxypropylated
 glycerol, and hexamethylene diisocyanate uretdione 352205-41-5P
 352205-43-7P 353244-60-7P, Castomer E 1004 353245-35-9P
 353245-36-0P

(preparation of two component polyurethane foam compns. for sound
 and vibration absorbers)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L50 ANSWER 6 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:439337 HCAPLUS

DOCUMENT NUMBER: 131:89112

TITLE: Reducing volatile organic content of coating
 compositions by using a ketimine of acetone

INVENTOR(S): Richards, Bradley M.; Dantiki, Sudhakar

PATENT ASSIGNEE(S): BASF Corporation, USA

SOURCE: U.S., 5 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

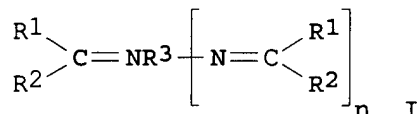
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5922804	A	19990713	US 1996-672800	1996 0628

PRIORITY APPLN. INFO.: US 1996-672800

1996
0628

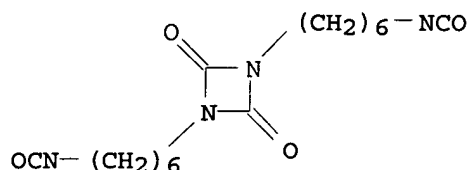
GI



AB The volatile organic content of coating compns. is reduced by forming the ketimine of acetone by reacting acetone and a ketimine I, where n = 1-4; R₁, R₂ are (sep.) alkyl, aryl, cycloaliph. or substituted alkyl, aryl, or cycloaliph. group, except both R₁ and R₂ ≠ Me; R₃ is an aliphatic, aromatic, arylaliph., or cycloaliph. group, which can also contain O, N, S or Si. The ketimine of acetone is subsequently reacted with at least one isocyanate functional crosslinking resin. Thus, 62.2 g uretdione polyisocyanate was added to a 50:50 solution of diketimine and acetone, and the coating sprayed on cold-rolled

steel panels, giving dry film thickness 2.6 mil, dust-free drying time 60 s, and tack-free drying time 105 s.

- IT 23501-81-7DP, Hexamethylene **diisocyanate** dimer, polymers with ketimines and hydroxy-functional resins (reducing volatile organic content of coating compns. by using a ketimine of acetone)
- RN 23501-81-7 HCAPLUS
- CN 1,3-Diazetidone-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



- IC ICM C08L075-02
ICS C08L075-04; C08G018-10
- INCL 524589000
- CC 42-5 (Coatings, Inks, and Related Products)
- ST coating VOC redn acetone ketimine; **isocyanate** crosslinker acetone ketimine polyol
- IT 23501-81-7DP, Hexamethylene **diisocyanate** dimer, polymers with ketimines and hydroxy-functional resins (reducing volatile organic content of coating compns. by using a ketimine of acetone)
- IT 584-84-9D, Toluene 2,4-**diisocyanate**, polymers with ketimines and hydroxy-functional resins 822-06-0D, HMDI, polymers with ketimines and hydroxy-functional resins 1014-98-8D, p-Xylene **diisocyanate**, polymers with ketimines and hydroxy-functional resins 3173-72-6D, 1,5-Naphthalene **diisocyanate**, polymers with ketimines and hydroxy-functional resins 3634-83-1D, m-Xylylene **diisocyanate**, polymers with ketimines and hydroxy-functional resins 4098-71-9D, Isophorone **diisocyanate**, polymers with ketimines and hydroxy-functional resins 5124-30-1D, 4,4'-**Diisocyanatodicyclohexylmethane**, polymers with ketimines and hydroxy-functional resins 10581-16-5D, 1-Methyl-2,4-**diisocyanatocyclohexane**, polymers with ketimines and hydroxy-functional resins 25626-25-9D, Benzene, 1,2-bis(**isocyanatomethyl**)-, polymers with ketimines and hydroxy-functional resins (reducing volatile organic content of coating compns. by using a ketimine of acetone)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 7 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:157156 HCAPLUS

DOCUMENT NUMBER: 130:244437

TITLE: Electrophotographic toner containing **polyisocyanate**

INVENTOR(S): Ibuki, Ichiro; Hamatsu, Takao

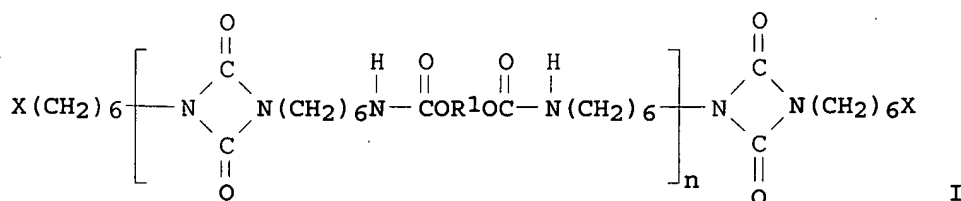
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

DOCUMENT TYPE: CODEN: JKXXAF
 LANGUAGE: Patent
 FAMILY ACC. NUM. COUNT: 1 Japanese
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11065169	A2	19990305	JP 1997-219483	1997 0814
PRIORITY APPLN. INFO.:			JP 1997-219483	1997 0814

GI

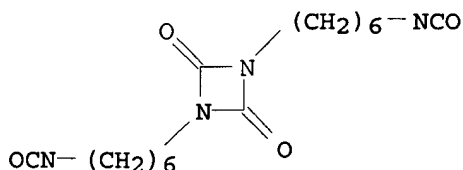


AB The toner comprises a polyol resin and a colorant as a main component and further a **polyisocyanate** containing a linear crystalline polyuretodione I [X = NHCO₂R₂OH, NHC(O)R₃, NCO; R₁ = R₂, R₂O₂CNHR₄NHCO₂R₂; R₂ = diol residue; R₃ = residue of a compound having 1 active H; R₄ = **diisocyanate** residue; n ≥ 1] with 8-21 weight% of potential NCO%, 2000-20,000 weight average mol. weight, and 60-140° m.p. The toner shows low **temperature** fixability and no offset.

IT 23501-81-7DP, polymer with ethylene glycol and polyester-polyol (electrophotog. toner containing polyuretodione-derived **polyurethanes** with low **temperature** fixability and offset resistance)

RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



IC ICM G03G009-087

CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 35

ST electrophotog toner **polyisocyanate** polyol

- polyuretodione; low temp fixability offset resistance toner
- IT Electrophotographic toners
(electrophotog. toner containing polyuretodione-derived **polyurethanes** with low **temperature** fixability and offset resistance)
- IT **Polyurethanes**, uses
(electrophotog. toner containing polyuretodione-derived **polyurethanes** with low **temperature** fixability and offset resistance)
- IT Acrylic polymers, preparation
(hydroxy-containing, polymer with polyuretodione; electrophotog. toner containing polyuretodione-derived **polyurethanes** with low **temperature** fixability and offset resistance)
- IT Polyesters, preparation
(polymers with hexamethylene **diisocyanate** polyuretodiones and ethylene glycol; electrophotog. toner containing polyuretodione-derived **polyurethanes** with low **temperature** fixability and offset resistance)
- IT 100-42-5DP, Styrene, hydroxy-containing acrylic resin, polymer with polyuretodione 107-21-1DP, Ethylene glycol, polymer with hexamethylene **diisocyanate** polyuretodione and polyester-polyols 23501-81-7DP, polymer with ethylene glycol and polyester-polyol
(electrophotog. toner containing polyuretodione-derived **polyurethanes** with low **temperature** fixability and offset resistance)

L50 ANSWER 8 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:126953 HCAPLUS

DOCUMENT NUMBER: 130:183894

TITLE: Method for preparing (poly)**isocyanate** compositions with reduced viscosity and their use in the manufacture of **polyurethane** coatings

INVENTOR(S): Charriere, Eugenie; Bernard, Jean-Marie; Revelant, Denis; Randu, Stephane

PATENT ASSIGNEE(S): Rhodia Chimie, Fr.

SOURCE: PCT Int. Appl., 67 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9907765	A1	19990218	WO 1998-FR1800	1998 0812
<p>W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW</p> <p>RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG</p>				
FR 2767328	A1	19990219	FR 1997-10296	

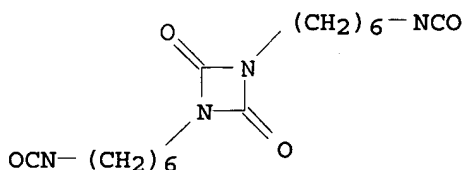
				1997 0812
FR 2767328	B1	20010622		
FR 2779142	A1	19991203	FR 1998-6849	
				1998 0529
FR 2779142	B1	20000818		
CA 2301071	AA	19990218	CA 1998-2301071	
				1998 0812
AU 9890758	A1	19990301	AU 1998-90758	
				1998 0812
AU 757808	B2	20030306		
ZA 9807209	A	20000214	ZA 1998-7209	
				1998 0812
EP 1003802	A1	20000531	EP 1998-942735	
				1998 0812
EP 1003802	B1	20041222		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,				
MC, PT, IE, FI				
BR 9811904	A	20000815	BR 1998-11904	
				1998 0812
EP 1466931	A2	20041013	EP 2004-14335	
				1998 0812
EP 1466931	A3	20051102		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,				
MC, PT, IE, FI, CY				
AT 285426	E	20050115	AT 1998-942735	
				1998 0812
ES 2230713	T3	20050501	ES 1998-942735	
				1998 0812
US 2004106762	A1	20040603	US 2003-682412	
				2003 1010
PRIORITY APPLN. INFO.:			FR 1997-10296	A
				1997 0812
			FR 1998-6849	A
				1998 0529
			EP 1998-942735	A3
				1998 0812
			WO 1998-FR1800	W
				1998 0812
			US 2000-485533	A1
				2000 0609

AB The invention concerns a method for preparing a (poly) **isocyanate** composition with reduced viscosity comprising at least dimers with uretidinedione group from initial monomeric **isocyanates**, characterized in that the initial reaction medium is **heated**, in the absence of a dimerization catalyst, at 50-200° for ≤24 h. When trimerization catalysts are present, the products also contain trimers, and, when polyols such as pentaerythritol and trimethylolpropane are present, the products contain carbamate group-containing prepolymers. The products are storage stable and have Hazen color value <100.

IT 23501-81-7P, Hexamethylene diisocyanate dimer
(preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)

RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)

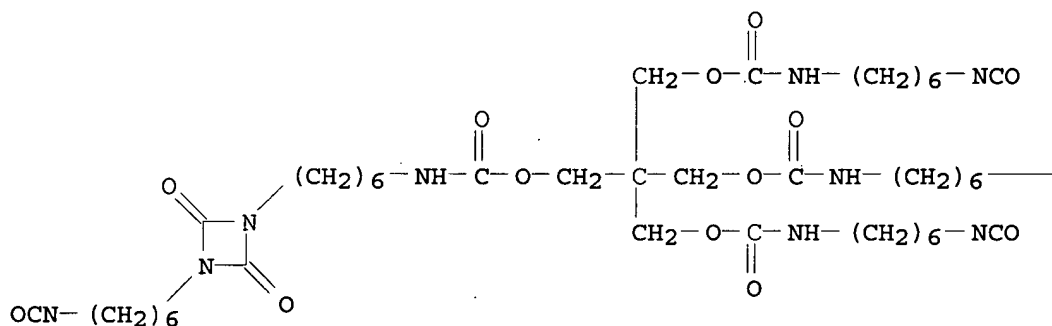


IT 220588-32-9P
(preparing **polyisocyanate** compns. containing **diisocyanate** dimers with reduced viscosity for use in manufacture of **polyurethane** coatings)

RN 220588-32-9 HCAPLUS

CN Carbamic acid, (6-isocyanatohexyl)-, 2-[[[(6-isocyanatohexyl)amino]carbonyl]oxy]methyl]-2-[[[(6-[3-(6-isocyanatohexyl)-2,4-dioxo-1,3-diazetidin-1-yl]hexyl]amino]carbonyl]oxy]methyl]-1,3-propanediyl ester (9CI)
(CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— NCO

IC ICM C08G018-79
ICS C08G018-32; C08G018-42; C08G018-62
CC 42-10 (Coatings, Inks, and Related Products)
ST uretidinedione **diisocyanate** dimer manuf dimerization
catalyst absence; trimethylolpropane uretidinedione dimer adduct
manuf; pentaerythritol uretidinedione dimer adduct manuf;
polyurethane coating uretidinedione **diisocyanate**
dimer precursor manuf
IT **Polyurethanes**, uses
(acrylic; preparing **polyisocyanate** compns. containing
diisocyanate dimers with reduced viscosity for use in
manufacture of **polyurethane** coatings)
IT Acrylic polymers, uses
(**polyurethane**-; preparing **polyisocyanate**
compns. containing **diisocyanate** dimers with reduced
viscosity for use in manufacture of **polyurethane** coatings)
IT Coating materials
(preparing **polyisocyanate** compns. containing
diisocyanate dimers with reduced viscosity for use in
manufacture of **polyurethane** coatings)
IT **Polyurethanes**, uses
(preparing **polyisocyanate** compns. containing
diisocyanate dimers with reduced viscosity for use in
manufacture of **polyurethane** coatings)
IT 220652-25-5P 220652-27-7P
(cured coating; preparing **polyisocyanate** compns. containing
diisocyanate dimers with reduced viscosity for use in
manufacture of **polyurethane** coatings)
IT 30228-08-1P
(in preparation of IPDI dimer; preparing **polyisocyanate**
compns. containing **diisocyanate** dimers with reduced
viscosity for use in manufacture of **polyurethane** coatings)
IT 53895-31-1P
(preparing **polyisocyanate** compns. containing
diisocyanate dimers with reduced viscosity for use in
manufacture of **polyurethane** coatings)
IT 3779-63-3P, Hexamethylene **diisocyanate** trimer
23501-81-7P, Hexamethylene **diisocyanate** dimer
(preparing **polyisocyanate** compns. containing
diisocyanate dimers with reduced viscosity for use in
manufacture of **polyurethane** coatings)
IT 4035-89-6P 220588-31-8P 220588-32-9P 220588-33-0P
220617-22-1P, 1,3-Bis(**isocyanatonorbornyl**
) -1,3-diazetidene-2,4-dione
(preparing **polyisocyanate** compns. containing
diisocyanate dimers with reduced viscosity for use in
manufacture of **polyurethane** coatings)
IT 30322-28-2P, Hexamethylene **diisocyanate**
-trimethylolpropane copolymer

(prepolymers, in preparation of HDI dimer; preparing polyisocyanate compns. containing diisocyanate dimers with reduced viscosity for use in manufacture of polyurethane coatings)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 9 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:379199 HCAPLUS

DOCUMENT NUMBER: 129:55022

TITLE: Uretdione group-containing polyaddition compounds and procedure for their production

INVENTOR(S): Gras, Rainer; Wolf, Elmar

PATENT ASSIGNEE(S): Huels A.-G., Germany

SOURCE: Ger. Offen., 6 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 19650043	A1	19980604	DE 1996-19650043	1996 1203

PRIORITY APPLN. INFO.: DE 1996-19650043

1996
1203

AB Title compds., useful as storage-stable curing agents for polyurethane powders, are manufactured by reaction of uretdiones of HDI, 2-methylpentamethylene diisocyanate, or 2,2,4(2,4,4)-trimethylhexamethylene diisocyanate with R1NHROH [I, R1 = H or C1-6 alkyl, R = (1-3-Me-substituted) C2-12 alkylene, (1-3-Me-substituted) C≤12 cycloalkylene] at 0.5 mol I/NCO equiv and optionally with monoamines and(or) alcs. at NCO:OH/NH 1:0.1-0.3 in an inert solvent.

IT 208587-38-6DP, reaction products with dibutylamine
208587-38-6P 208594-47-2DP, reaction products
with butanol 208594-49-4P 208666-50-6P
(polyaddn. compds. of uretdione group-containing diisocyanate dimers and amino alcs. for crosslinkers for polyurethane powders)

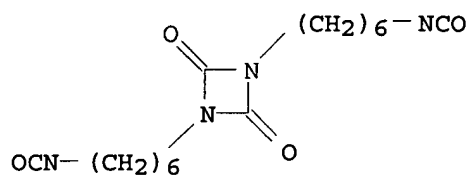
RN 208587-38-6 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with 2-aminoethanol (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

CMF C16 H24 N4 O4



CM 2

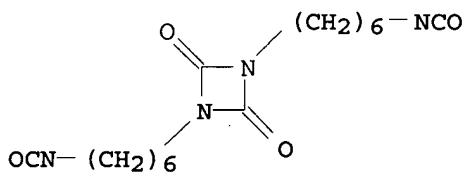
CRN 141-43-5
CMF C2 H7 N O

H₂N-CH₂-CH₂-OH

RN 208587-38-6 HCAPLUS
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer
with 2-aminoethanol (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7
CMF C16 H24 N4 O4



CM 2

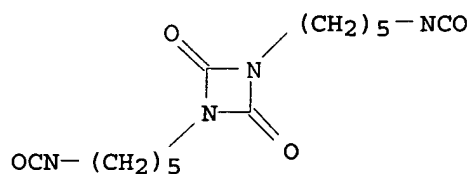
CRN 141-43-5
CMF C2 H7 N O

H₂N-CH₂-CH₂-OH

RN 208594-47-2 HCAPLUS
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(5-isocyanatomethylpentyl)-,
polymer with 2-(methylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 208594-46-1
CMF C16 H24 N4 O4
CCI IDS



2 (D1-Me)

CM 2

CRN 109-83-1

CMF C3 H9 N O



RN 208594-49-4 HCAPLUS

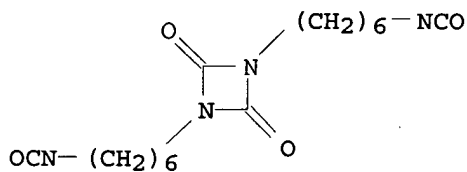
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with 2-aminoethanol (9CI) (CA INDEX NAME)

CM 1

CRN 208594-48-3

CMF C22 H36 N4 O4

CCI .IDS

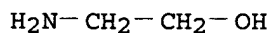


6 (D1-Me)

CM 2

CRN 141-43-5

CMF C2 H7 N O



RN 208666-50-6 HCAPLUS

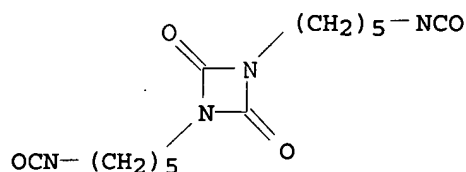
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(5-isocyanato-2(or 4)-methylpentyl)-, polymer with 1-amino-2-propanol (9CI) (CA INDEX NAME)

CM 1

CRN 208594-46-1

CMF C16 H24 N4 O4

CCI IDS

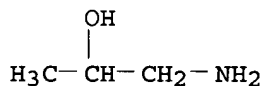


2 (D1-Me)

CM 2

CRN 78-96-6

CMF C3 H9 N O



IC ICM C08G018-79

ICS C08G018-32; C09D175-04; C09D005-46; C08L075-04

CC 37-6 (Plastics Manufacture and Processing)

ST uretdione **diisocyanate** amino alc polyadduct manuf;

polyurethane powder latent crosslinker

IT Crosslinking agents

(latent; polyaddn. compds. of uretdione group-containing **diisocyanate** dimers and amino alcs. for crosslinkers for **polyurethane** powders)

IT **Polyurethanes**, uses

(polyaddn. compds. of uretdione group-containing **diisocyanate** dimers and amino alcs. for crosslinkers for **polyurethane** powders)

IT **Polyurethanes**, preparation

Polyurethanes, preparation

(polyurea-; polyaddn. compds. of uretdione group-containing **diisocyanate** dimers and amino alcs. for crosslinkers for **polyurethane** powders)

IT Polyureas

Polyureas

(**polyurethane**-; polyaddn. compds. of uretdione group-containing **diisocyanate** dimers and amino alcs. for crosslinkers for **polyurethane** powders)

IT Alcohols, preparation

Amines, preparation

(reaction products, with uretdione group-containing **diisocyanate**-amino alcs. copolymers; polyaddn. compds. of uretdione group-containing **diisocyanate** dimers and

amino alcs. for crosslinkers for **polyurethane** powders)

IT 71-36-3DP, 1-Butanol, reaction products with uretdione group-containing **diisocyanate** dimer-amino alcs. copolymers, preparation 111-92-2DP, Dibutylamine, reaction products with uretdione group-containing **diisocyanate** dimer-amino alcs. copolymers 208587-38-6DP, reaction products with dibutylamine 208587-38-6P 208587-39-7DP, reaction products with dibutylamine 208587-39-7P 208594-47-2DP, reaction products with butanol 208594-49-4P 208666-50-6P

(polyaddn. compds. of uretdione group-containing **diisocyanate** dimers and amino alcs. for crosslinkers for **polyurethane** powders)

L50 ANSWER 10 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:15965 HCAPLUS

DOCUMENT NUMBER: 128:89733

TITLE: Microcapsules with walls from conversion products of uretdione group-containing **polyisocyanates** and guanidine derivatives

INVENTOR(S): Hagedorn, Manfred; Nehen, Ulrich; Ramzy, Sabry; Klug, Guenter; Weisser, Juergen

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Ger. Offen., 10 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

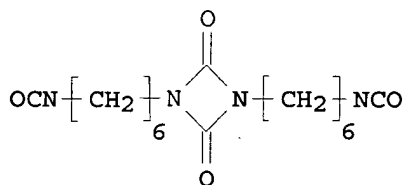
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 19623566	A1	19971218	DE 1996-19623566	

1996
0613

PRIORITY APPLN. INFO.: DE 1996-19623566

1996
0613

GI



I

AB Microcapsules with high d. and good storage stability, useful for carbonless copying paper, have walls prepared by reaction of the title compds. Typical microcapsules were manufactured by mixing a 10% aqueous guanidine carbonate solution with an emulsion containing crystal violet lactone, diisopropylnaphthalene, polyvinyl alc., and a

60:40 **diisocyanate** I-OCN(CH₂)₆NHCON[(CH₂)₆NCO]CONH(CH₂)₆
NCO mixture 90 min at 80°.

IT 200507-27-3P

(microcapsules with walls from conversion products of uretdione
group-containing **polyisocyanates** and guanidine derivs.
for carbonless copying paper)

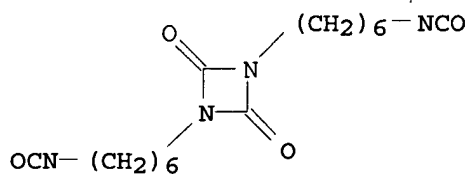
RN 200507-27-3 HCAPLUS

CN Carbonic acid, compd. with guanidine (1:2), polymer with
1,3-bis(6-isocyanatohexyl)-1,3-diazetidine-2,4-dione and
N,N',2-tris(6-isocyanatohexyl)imidodicarbonic diamide (9CI) (CA
INDEX NAME)

CM 1

CRN 23501-81-7

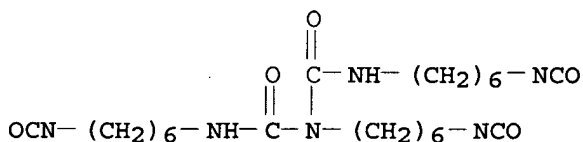
CMF C16 H24 N4 O4



CM 2

CRN 4035-89-6

CMF C23 H38 N6 O5



CM 3

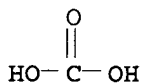
CRN 593-85-1

CMF C H5 N3 . 1/2 C H2 O3

CM 4

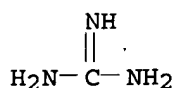
CRN 463-79-6

CMF C H2 O3



CM 5

CRN 113-00-8
CMF C H5 N3



IC ICM B01J013-16
ICA B41M005-165
CC 38-3 (Plastics Fabrication and Uses)
Section cross-reference(s): 74
ST microcapsule guanidine uretdione contg polyurea; carbonless
copying paper microcapsule polyurea; **hexanediisocyanate**
based uretdione contg polyurea microcapsule
IT Copying paper
Microcapsules
(microcapsules with walls from conversion products of uretdione
group-containing **polyisocyanates** and guanidine derivs.
for carbonless copying paper)
IT Polyureas
(uretdione-containing; microcapsules with walls from conversion
products of uretdione group-containing **polyisocyanates**
and guanidine derivs. for carbonless copying paper)
IT 200507-27-3P
(microcapsules with walls from conversion products of uretdione
group-containing **polyisocyanates** and guanidine derivs.
for carbonless copying paper)

L50 ANSWER 11 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:632095 HCAPLUS
DOCUMENT NUMBER: 127:248526
TITLE: Polyaddition products of dissecondary diamines
and **polyisocyanate** mixtures
containing uretdione groups
INVENTOR(S): Wolf, Elmar
PATENT ASSIGNEE(S): Huels Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 7 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 795569	A1	19970917	EP 1997-100842	1997 0121
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE DE 19610465	A1	19970918	DE 1996-19610465	1996 0316
JP 10036483	A2	19980210	JP 1997-58184	1997 0313
CA 2200044	AA	19970916	CA 1997-2200044	1997

US 5912314

A

19990615

US 1997-819365

0314

1997

0317

PRIORITY APPLN. INFO.:

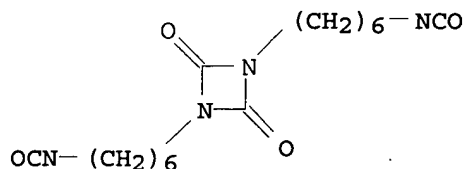
DE 1996-19610465

A

1996

0316

- AB The title products, useful as curing agents for **polyurethanes** (e.g., powder coatings) (no data), are prepared from uretdione derivative **polyisocyanates** [≥ 40 mol% IPDI uretdione **diisocyanate**] and dissecondary diamines (NCO-NH ratio 1:0.5-0.9) at room temp -60° in inert solvents. Reaction of 3 equivalent N,N'-bis[3-methyl-1-(3-methylpropyl)butyl]-2,2 (or 4),4-trimethyl-1,6-hexanediamine (prepared in $>98\%$ purity by reductive amination of the diprimary diamine with iso-Bu₂CO) with 4 equivalent 1:1 mixture of HMDI and IPDI uretdione derivative **diisocyanates** gave a product with m.p. $68-81^\circ$ and NCO content 2.6 and 12.5% before and after, resp., being heated at 180° .
- IT 23501-81-7DP, 1,3-Bis(6-isocyanatohexyl)-2,4-uretedione, reaction products with dissecondary diamines (polyaddn. products of dissecondary diamines and **polyisocyanate** mixts. containing uretdione groups)
- RN 23501-81-7 HCAPLUS
- CN 1,3-Diazetidione-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



- IC ICM C08G018-79
ICS C08G018-32; C08G018-80
- CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27
- ST diamine dissecondary adduct **diisocyanate**; uretdione **diisocyanate** adduct diamine; HMDI uretdione adduct diamine; IPDI uretdione adduct diamine; crosslinker **polyurethane** powder coating
- IT Crosslinking agents
(adducts of dissecondary diamines and uretdione **diisocyanates** as crosslinking agents for **polyurethane** powder coatings)
- IT **Polyurethanes**, uses
(adducts of dissecondary diamines and uretdione **diisocyanates** as crosslinking agents for **polyurethane** powder coatings)
- IT Amines, preparation
(diamines, dissecondary, reaction products with uretdione **diisocyanates**; polyaddn. products of dissecondary diamines and **polyisocyanate** mixts. containing uretdione groups)
- IT Coating materials

(powder; adducts of disecundary diamines and uretdione diisocyanates as crosslinking agents for polyurethane powder coatings)

IT 192528-25-9DP, reaction products with uretdione diisocyanates
(polyaddn. products of disecundary diamines and polyisocyanate mixts. containing uretdione groups)

IT 23501-81-7DP, 1,3-Bis(6-isocyanatohexyl)-2,4-uretdione, reaction products with disecundary diamines 41094-42-2DP, N,N'-Diisobutylisophoronediamine, reaction products with uretdione diisocyanates 53895-31-1DP, IPDI dimer, uretdione group-containing, reaction products with disecundary diamines 192462-35-4DP, reaction products with uretdione diisocyanates 192528-26-0DP, reaction products with uretdione diisocyanates
(polyaddn. products of disecundary diamines and polyisocyanate mixts. containing uretdione groups)

L50 ANSWER 12 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:513130 HCAPLUS
DOCUMENT NUMBER: 125:144831
TITLE: One component-type fast heat-curable polyurethane elastomer compositions and their molding method
INVENTOR(S): Hirayama, Shinji; Konishi, Shin; Hashimoto, Sadako; Morikawa, Yukihiro
PATENT ASSIGNEE(S): Inoue MTP KK, Japan; Nippon Polyurethane Kogyo KK; Nippon Polyurethane Industry Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08134164	A2	19960528	JP 1994-306908	1994 1115
JP 3509967	B2	20040322	JP 1994-306908	1994 1115

PRIORITY APPLN. INFO.:

AB The title compns. comprise (1) polyurethane precursors with equivalent ratio of uretdione group to active H (r-1) 0.25-1.0 prepared by treating (A) polyisocyanates at least containing polyisocyanates with uretdione groups and (B) ≥ 2 active H-containing compds. with mol. weight 18-20,000 at equivalent ratio of the active H to the NCO (r-2) > 1.0 and (2) 1,5-diazabicyclo[4.3.0]nonene-5 (DBN) and/or their salts. The title molding method comprises injecting the compns. at a temperature lower or equal to the ring-opening temperature of the uretdione group (T), molding, and heating at a temperature higher or equal to T for reacting and curing. Thus, 100 parts a composition comprising a precursor with r-1 0.72 prepared by treating uretdione group-containing HDI derivative and polytetramethylene ether polyol at ratio r-2 1.3, 0.5 part DBN, and 0.5 part Irganox 1010 were fed to a reactor and stirred at 80° to give a composition, which was

press molded and cured at 200°.

IT 180163-58-0P
(rubber; one component-type fast heat-curable polyurethane elastomer compns. and their molding method)

RN 180163-58-0 HCAPLUS

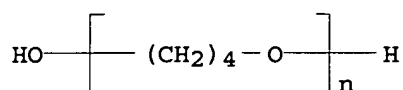
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with α -hydro- ω -hydroxypoly(oxy-1,4-butanediyl) (9CI)
(CA INDEX NAME)

CM 1

CRN 25190-06-1

CMF (C4 H8 O)_n H2 O

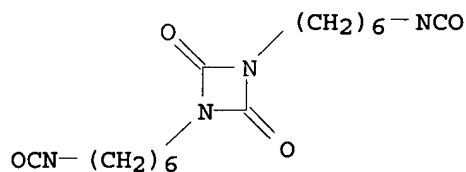
CCI PMS



CM 2

CRN 23501-81-7

CMF C16 H24 N4 O4



IC ICM C08G018-10

ICS C08G018-20; C08G018-70; C08G018-79

CC 39-9 (Synthetic Elastomers and Natural Rubber)

IT 180163-58-0P
(rubber; one component-type fast heat-curable polyurethane elastomer compns. and their molding method)

L50 ANSWER 13 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:209693 HCAPLUS

DOCUMENT NUMBER: 124:235011

TITLE: Liquid polyisocyanates containing aromatic and aliphatic isocyanate groups for use in lacquers

INVENTOR(S): Brahm, Martin; Pedain, Josef; Schmalstieg, Lutz

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Eur. Pat. Appl., 8 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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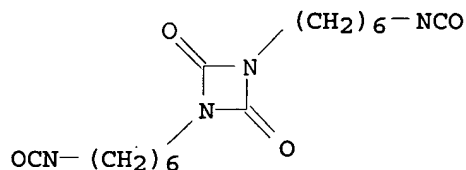
EP 696606	A1	19960214	EP 1995-111814	1995 0727
EP 696606	B1	19991124		
R: AT, BE, DE, ES, FR, GB, IT, NL				
DE 4428107	A1	19960215	DE 1994-4428107	1994 0809
AT 186928	E	19991215	AT 1995-111814	1995 0727
ES 2139791	T3	20000216	ES 1995-111814	1995 0727
US 5606004	A	19970225	US 1995-509258	1995 0731
CA 2155473	AA	19960210	CA 1995-2155473	1995 0804
JP 08059771	A2	19960305	JP 1995-219446	1995 0807
JP 3604204	B2	20041222		
PRIORITY APPLN. INFO.:			DE 1994-4428107	A 1994 0809

AB The title **polyisocyanates** are prepared by mixed trimerization of TDI (optionally containing other aromatic **isocyanates**) with aliphatic **isocyanates** (e.g., uretedione group-containing dimer of HDI). The **polyisocyanates** are especially useful as crosslinkers for OH-containing binders in two-component **polyurethane** lacquers.

IT **23501-81-7DP**, 1,3-Bis(6-**isocyanato**hexyl)-1,3-diazetidione-2,4-dione, reaction products with TDI (liquid; preparation and use as crosslinkers for two-component **polyurethane** lacquers)

RN **23501-81-7** HCAPLUS

CN 1,3-Diazetidione-2,4-dione, 1,3-bis(6-**isocyanato**hexyl)- (9CI) (CA INDEX NAME)



IC ICM C08G018-79
ICS C08G018-02
CC 42-10 (Coatings, Inks, and Related Products)
ST liq aliph arom **polyisocyanate** crosslinker
polyurethane; TDI HDI **polyisocyanate** liq
crosslinker **polyurethane**; lacquer **polyurethane**

crosslinker liq **polyisocyanate**
 IT Coating materials
 (liquid **polyisocyanates** prepared from aromatic and aliphatic
 isocyanates for use as hardeners in two-component
 polyurethane lacquers)
 IT **Urethane** polymers, uses
 (liquid **polyisocyanates** prepared from aromatic and aliphatic
 isocyanates for use as hardeners in two-component
 polyurethane lacquers)
 IT Crosslinking agents
 (liquid **polyisocyanates** prepared from aromatic and aliphatic
 isocyanates for use in two-component
 polyurethane lacquers)
 IT 584-84-9DP, 2,4-Tdi, reaction products with aliphatic
 polyisocyanates 26471-62-5DP, TDI, reaction products
 with aliphatic **polyisocyanates**
 (liquid; preparation and as crosslinkers for two-component
 polyurethane lacquers)
 IT 23501-81-7DP, 1,3-Bis(6-**isocyanatohexyl**
)-1,3-diazetidione-2,4-dione, reaction products with TDI
 28574-90-5DP, Hexamethylene **diisocyanate** trimer,
 reaction products with TDI
 (liquid; preparation and use as crosslinkers for two-component
 polyurethane lacquers)

L50 ANSWER 14 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:130831 HCAPLUS

DOCUMENT NUMBER: 124:205122

TITLE: Coating compositions containing aldimines and
isocyanates

INVENTOR(S): Braun, David W.; Colyer, Emmerson Keith;
 Dantiki, Sudhakar; Tye, Anthony J.; Shah,
 Rajnikant P.; Mormile, Patrick J.; Richards,
 Bradley M.; Koevenig, Brian P.; Laginess,
 Thomas J.; Stateczny, Henry J.

PATENT ASSIGNEE(S): BASF Corp., USA

SOURCE: Eur. Pat. Appl., 27 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 686654	A1	19951213	EP 1995-107978	1995 0526
EP 686654	B1	20031001		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
AT 251190	E	20031015	AT 1995-107978	1995 0526
ES 2208660	T3	20040616	ES 1995-107978	1995 0526
AU 9520459	A1	19951214	AU 1995-20459	1995 0602

AU 701598	B2	19990204			
CA 2151014	AA	19951207	CA 1995-2151014		1995 0605
BR 9502671	A	19970805	BR 1995-2671		1995 0605
JP 08060089	A2	19960305	JP 1995-162929		1995 0606
ZA 9504597	A	19961205	ZA 1995-4597		1996 0605
AU 9888361	A1	19981203	AU 1998-88361		1998 1008
AU 736624	B2	20010802			
PRIORITY APPLN. INFO.:			US 1994-254211	A	1994 0606
			AU 1995-20459	A3	1995 0602

AB High-solids compns. with good pot life for coatings contain (a) (R1CH:N)nR2 [R1 = (substituted) alkyl, (substituted) aryl, (substituted) cycloalkyl, substituted heterocyclic group, R2 = monomeric or polymeric aliphatic, aromatic, arylaliph. or cycloaliph. group which may contain O, N, S, or Si, n > 1], (b) a **polyisocyanate** functional component, and (c) optionally, other active hydrogen compds. A typical composition contained 1:2 (mol ratio) isophoronediamine-isobutylaldehyde adduct 72.56, catalyst 0.82, HDI uretdione 90.88, and flow modifier and photostabilizers 5.75 parts.

IT 173923-56-3P 174423-54-2P

(high-solids compns. containing aldimines and **polyisocyanates** with good pot life for coatings)

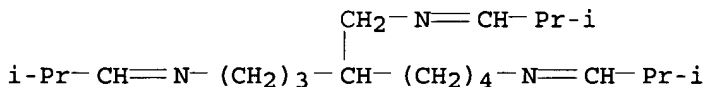
RN 173923-56-3 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with N,N'-bis(2-methylpropylidene)-4-[[2-methylpropylidene)amino]methyl]-1,8-octanediamine (9CI) (CA INDEX NAME)

CM 1

CRN 173923-55-2

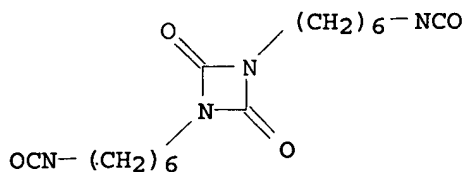
CMF C21 H41 N3



CM 2

CRN 23501-81-7

CMF C16 H24 N4 O4



RN 174423-54-2 HCAPLUS

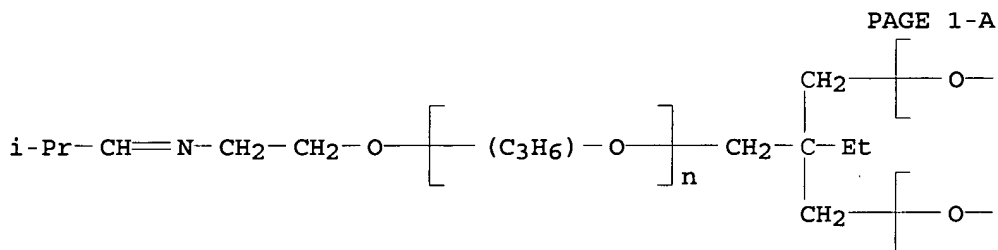
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with α -hydro- ω -[methyl-2-[(2-methylpropylidene)amino]ethoxy]poly[oxy(methyl-1,2-ethanediyl)] ether with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (3:1) (9CI) (CA INDEX NAME)

CM 1

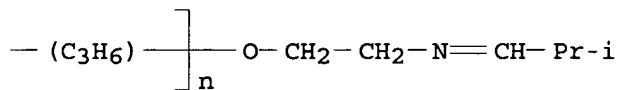
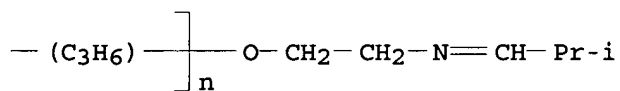
CRN 174423-53-1

CMF (C3 H6 O)_n (C3 H6 O)_n (C3 H6 O)_n C27 H53 N3 O3

CCI IDS, PMS



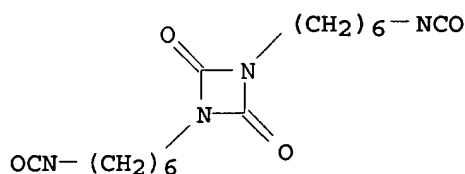
3 (D1-Me)



CM 2

CRN 23501-81-7

CMF C16 H24 N4 O4



IC ICM C08G018-32
ICS C08G018-79; C09D017-00; C09D007-02; C07C251-16
CC 42-10 (Coatings, Inks, and Related Products)
ST **polyisocyanate** aldimine copolymer coating; storage
stable **polyisocyanate** aldimine coating; isophorone
bisisobutylidimine HDI uretdione copolymer coating
IT Polyamides, uses
(imine-group-containing; high-solids compns. containing aldimines and
polyisocyanates with good pot life for coatings)
IT Coating materials
(high-solids, high-solids compns. containing aldimines and
polyisocyanates with good pot life for coatings)
IT Polyisocyanurates
(polyamide-, imine- and uretdione-group-containing; high-solids
compns. containing aldimines and **polyisocyanates** with
good pot life for coatings)
IT Polyamides, uses
(polyisocyanurate-, imine- and uretdione-group-containing;
high-solids compns. containing aldimines and
polyisocyanates with good pot life for coatings)
IT 173923-54-1P 173923-56-3P 173923-58-5P 173923-60-9P
173923-61-0P 173923-62-1P 174423-54-2P 174587-94-1P
(high-solids compns. containing aldimines and
polyisocyanates with good pot life for coatings)

L50 ANSWER 15 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:633093 HCAPLUS

DOCUMENT NUMBER: 121:233093

TITLE: New aliphatic polyisocyanate curing agents for
higher solids urethane coatings

AUTHOR(S): Wojcik, R. T.; Goldstein, S. L.; Malofsky, A.
G.; Barnowski, H. G., Jr.; Chandalia, K. B.

CORPORATE SOURCE: Chem. Res. Cent., Olin Corp., Cheshire, CT,
06410, USA

SOURCE: Proceedings of the Waterborne, High-Solids,
and Powder Coatings Symposium (1993), 20th,
26-48

CODEN: PWHSE6

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Polyisocyanate curing agents prepared from hexamethylene
diisocyanate (HDI) are used com. in High Solids Paints for
automotive, maintenance, and industrial finishes. These products
are based on isocyanurate or biuret chemical Olin has an active
research program to develop low viscosity polyisocyanates. In
this program, the authors made very pure HDI isocyanurate trimer
and HDI uretidione cross-linkers and studied their effect on 2K
polyurethane coatings processing and performance. These curing
agents were formulated into High Solids Paints with com. available
polyols. Appearance VOC, paint coverage, coating appearance
(gloss & DOI), mech. performance (hardness, flexibility, and

impact), environmental durability (gloss retention, chalking, and cracking), and chemical/moisture resistance were compared to standard 2K polyurethane coatings formulated with com. HDI polyisocyanurate (LuxateTM HT2000). The coatings made with the new curing agent had lower VOC and superior appearance compared to the com. polyisocyanate. The mech. properties and environmental durability of the coatings were similar. Compared to the coatings made with LuxateTM HT2000, these curing agents had slower dry times and reduced surface hardness. This paper suggests formulation methods to decrease the dry times and increase surface hardness.

IT 158407-53-5 158407-54-6

(New aliphatic polyisocyanate curing agents for higher solids urethane coatings)

RN 158407-53-5 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with G-Cure 105P70 (9CI) (CA INDEX NAME)

CM 1

CRN 158191-40-3

CMF Unspecified

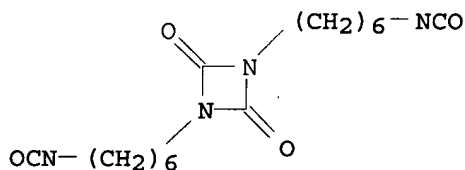
CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 23501-81-7

CMF C16 H24 N4 O4



RN 158407-54-6 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with Acryloid AU 946 and QM 1007 (9CI) (CA INDEX NAME)

CM 1

CRN 158191-13-0

CMF Unspecified

CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 115628-82-5

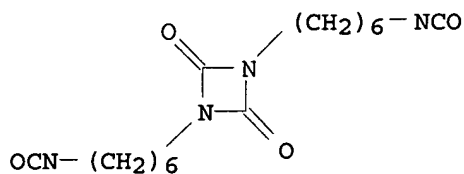
CMF Unspecified

CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 3

CRN 23501-81-7
CMF C16 H24 N4 O4



CC 42-3 (Coatings, Inks, and Related Products)
IT 158407-53-5 158407-54-6
(New aliphatic polyisocyanate curing agents for higher solids urethane coatings)

L50 ANSWER 16 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:484214 HCAPLUS

DOCUMENT NUMBER: 121:84214

TITLE: Process for producing uretidione dimers of isocyanates using catalysts which are bound to inorganic matrixes

INVENTOR(S): Goldstein, Stephen L.; Hamer, Anthony D.; Katz, Lawrence E.; McGeary, Michael J.; Smith, Curtis P.

PATENT ASSIGNEE(S): Olin Corp., USA

SOURCE: U.S., 7 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

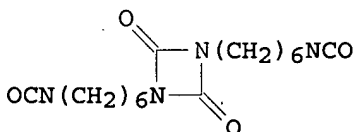
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	
US 5315004	A	19940524	US 1993-43075	1993 0405
US 5461020	A	19951024	US 1994-241249	1994 0511
PRIORITY APPLN. INFO.:			US 1993-43075	A2 1993 0405

GI

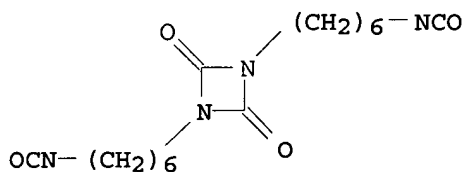


I

AB The invention relates to a process for preparing a dimer by

cyclodimerizing a **polyisocyanate** in the presence of a dimerization catalyst which is covalently bound to an insol. inorg. matrix. Said **polyisocyanate** is contacted with the catalyst at a **temperature** of between 20-135°C to form an uretidione (cyclodimerized **isocyanate**). Thus, silica-bound N,N-bis[3-(diethoxymethylsilyl)propyl]-4-pyridinamine was used as cyclodimerization catalyst for HDI. The IR spectrum of the products showed no absorption due to isocyanurates; 15% of HDI were converted to hexamethylene **diisocyanate** dimer [1,3-bis(6-**isocyanatohexyl**)-2,4-uretidinedione] (I).

IT 23501-81-7P, Hexamethylene **diisocyanate** dimer
(preparation of, with inorg. matrix-bound (dialkylamino)pyridine as cyclodimerization catalyst)
RN 23501-81-7 HCAPLUS
CN 1,3-Diazetidione-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



IC ICM C07D229-00
ICS C08G018-74
INCL 540202000
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 28
ST uretidione hexamethylene **diisocyanate** dimer;
cyclodimerization catalyst pyridinamine silica bound
IT Glass, nonoxide
(cyclodimerization catalyst-supports for **diisocyanate**)
IT Clays, uses
Zeolites, uses
(inorg. matrix-bound amines as cyclodimerization catalysts for **diisocyanates**)
IT Glass, oxide
(inorg. matrix-bound, cyclodimerization catalysts for **diisocyanate**)
IT Amines, uses
(aryl, inorg. matrix-bound, cyclodimerization catalysts for **diisocyanate**)
IT Dimerization catalysts
(cyclo-, inorg. matrix-bound (dialkylamino)pyridine for **isocyanates**)
IT Dimerization
(cyclo-, of **diisocyanates** with inorg. matrix-bound (dialkylamino)pyridine)
IT Amines, uses
(tertiary, inorg. matrix-bound, cyclodimerization catalysts for **diisocyanate**)
IT 128823-47-2D, 4-Pyridinamine, N,N-bis[3-(diethoxymethylsilyl)propyl]-, inorg. matrix-bound 129677-07-2D, 4-Pyridinamine, N-[(ethenylphenyl)methyl]-N-methyl-, inorg. matrix-bound
(as cyclodimerization catalyst for **diisocyanate**)

IT 1344-28-1, Aluminum oxide (Al₂O₃), uses 7631-86-9, Silica, uses
(inorg. matrix-bound amines as cyclodimerization catalysts for
diisocyanates)

IT 7803-51-2D, Phosphine, alkyl or alkylamino derivs.
(inorg. matrix-bound, cyclodimerization catalysts for
diisocyanate)

IT 23501-81-7P, Hexamethylene **diisocyanate** dimer
26747-90-0P, TDI dimer 53895-31-1P, IPDI dimer
(preparation of, with inorg. matrix-bound (dialkylamino)pyridine as
cyclodimerization catalyst)

L50 ANSWER 17 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:247474 HCAPLUS

DOCUMENT NUMBER: 120:247474

TITLE: Use of alkylthio-substituted aromatic diamines
as curing agents for **polyisocyanates**
in coating and sealing compositions

INVENTOR(S): Hentschel, Karl Heinz; Walter, Ulrich

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

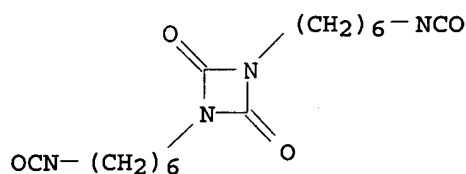
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	
EP 570798	A1	19931124	EP 1993-107559	1993 0510
R: CH, DE, ES, FR, GB, IT, LI, NL				
DE 4217023	A1	19931125	DE 1992-4217023	1992 0522
CA 2096466	AA	19931123	CA 1993-2096466	1993 0518
JP 06049410	A2	19940222	JP 1993-139886	1993 0520
PRIORITY APPLN. INFO.:			DE 1992-4217023	A 1992 0522

AB Arom diamines containing ≥ 1 C1-4 alkylthio group ortho to each
amino group, especially a mixture of 2,4- and 2,6-diamino-1-methyl-3,5-
bis(methylthio)benzenes, are used, optionally with other
polyamines and/or polyols, as hardeners for
polyisocyanates in 2-component coating or sealing compns.
which contain little or no solvent and cure at room temp
. without forming bubbles or voids.

IT 23501-81-7DP, Hexamethylene **diisocyanate** dimer,
polymers with alkylthio aromatic diamines and polyols
(preparation of, for two-component coating and sealing compns.)

RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidene-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA
INDEX NAME)



IC ICM C08G018-38
ICS C08G018-10; C09D175-02; C04B041-48; C09K003-10
CC 42-10 (Coatings, Inks, and Related Products)
ST amine arom alkylthio polyurea **polyurethane**; sulfide
amine arom polyurea **polyurethane**; crosslinking alkylthio
amine polyurea **polyurethane**; sealant polyurea
polyurethane alkylthio amine
IT Crosslinking agents
(diamines, aromatic, alkylthio, for polyurea-**polyurethanes**
in coatings and sealants)
IT **Urethane** polymers, preparation
(polyurea-, preparation of, for two-component coatings and sealants,
alkylthio aromatic diamines in)
IT Coating materials
Sealing compositions
(two-component, polyurea-**polyurethanes** for, alkylthio
aromatic diamine-containing)
IT 584-84-9DP, 2,4-Diisocyanatotoluene, polymers with
alkylthio aromatic diamines, and polyols 822-06-0DP, HDI, polymers
with alkylthio aromatic diamines and polyols 3779-63-3DP, polymers
with alkylthio aromatic diamines and polyols 5873-54-1DP, 2,4'-
Diisocyanatodiphenylmethane, polymers with alkylthio aromatic
diamines and polyols 9016-87-9DP, PAPI, polymers with alkylthio
aromatic diamines and polyols 23501-81-7DP, Hexamethylene
diisocyanate dimer, polymers with alkylthio aromatic diamines
and polyols 25322-69-4DP, Polypropylene glycol, polymers with
alkylthio aromatic diamines and **polyisocyanates**
25723-16-4DP, Polypropylene glycol trimethylolpropane ether,
polymers with alkylthio aromatic diamines and **polyisocyanates**
26471-62-5DP, Tdi, polymers with alkylthio aromatic diamines and
polyols 54511-70-5DP, polymers with alkylthio aromatic diamines and
polyisocyanates 102093-68-5DP, polymers with
polyisocyanates and polyols 104983-85-9DP, polymers with
polyisocyanates and polyols 106264-79-3DP, Ethacure 300,
polymers with **polyisocyanates** and polyols
107120-02-5DP, polymers with alkylthio aromatic diamines and
polyisocyanates
(preparation of, for two-component coating and sealing comps.)

L50 ANSWER 18 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:137262 HCAPLUS

DOCUMENT NUMBER: 120:137262

TITLE: Aqueous **polyurethane** binder
combination, process for its preparation and
its use

INVENTOR(S): Blum, Harald; Kubitz, Werner; Probst,
Joachim; Sonntag, Michael; Schneider, Volker

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Eur. Pat. Appl., 20 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

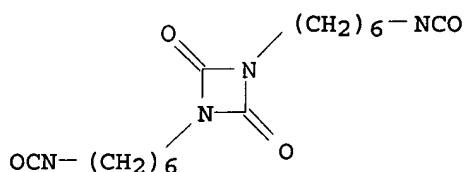
LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO. -----	KIND ----	DATE -----	APPLICATION NO. -----	DATE
EP 542105	A1	19930519	EP 1992-118831	1992 1103
EP 542105 R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE	B1	19960124		
DE 4137429	A1	19930519	DE 1991-4137429	1991 1114
AT 133430	E	19960215	AT 1992-118831	1992 1103
ES 2084909	T3	19960516	ES 1992-118831	1992 1103
US 5331039	A	19940719	US 1992-973368	1992 1109
CA 2082785	AA	19930615	CA 1992-2082785	1992 1112
JP 05295072	A2	19931109	JP 1992-326290	1992 1112
JP 2923718	B2	19990726		
KR 217448	B1	19990901	KR 1992-21281	1992 1113
PRIORITY APPLN. INFO.:			DE 1991-4137429	A 1991 1114

AB The title binders, useful for varnishes, coats, sealants, and adhesives with reduced organic solvent content, are obtained by mixing a **polyisocyanate** component and a H₂O-thinned polyester-polyol component which is a blend of ≥ 2 hydroxy-, **urethane-**, carboxy-, or sulfonate-containing (acrylate-grafted) polyester resins. An aqueous dispersion (A) of a polyester-urethane-polyol prepared from trimethylolpropane, isophthalic acid, saturated fatty acids (Prifrac 2950), neopentyl glycol, hexahydrophthalic anhydride, dimethylolpropionic acid, and isophorone **diisocyanate** had solids content 48.5%, pH 7.4 (NH₄OH), acid number 10, and OH group content 4.6%. Another aqueous dispersion (B) prepared by polymerization of 2-hydroxyethyl methacrylate, Me methacrylate, Bu acrylate, and acrylic acid in BuOAc solvent followed by emulsification of the polymer solution in H₂O with azeotropic removal of the solvent, had solids content 30%, pH 7.0 (NH₄OH), carboxy group content 139 mequiv/100 g solids, and OH group content 4.6%. A (storage-stable) blend containing A 50, B 50, thickener 1.14, emulsifier 0.8, defoamer 0.93, and deionized H₂O 4.9 parts was mixed with 28.88 parts solvent-free 70:30 HMDI dimer-HMDI trimer mixture (average NCO group content 22.5%, viscosity 200 mPa-s, 23°) to give a 2-component title binder having NCO/OH ratio

1.5 and open time .apprx.5 h. A 200- μ m (wet thickness) clear coat was dust-free dry after 2-3 h at room temperature and after 10-14 days had pendulum hardness 100-120 s.

IT 23501-81-7DP, Hexamethylene diisocyanate dimer, polymers with polyester polyols
(preparation of aqueous dispersions of, as binders)
RN 23501-81-7 HCAPLUS
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



IC ICM C08G018-42
ICS C08G018-40; C08G018-72; C08G018-08; C09D175-06
CC 42-10 (Coatings, Inks, and Related Products)
Section cross-reference(s): 37
ST polyester aq dispersion prepn **polyurethane** binder;
lacquer **polyurethane** aq polyester dispersion; HMDI dimer
trimer aq **polyurethane** binder
IT Binding materials
(aqueous **polyurethane** compns.)
IT Sealing compositions
(aqueous **polyurethane** compns. as)
IT Coating materials
(aqueous **polyurethane** compns. for)
IT Adhesives
(binders for, aqueous **polyurethane** compns. as)
IT Fatty acids, compounds
(C14-16, reaction products, with polyols and isophorone
isocyanate, preparation of, for aqueous **polyurethane**
binder compns.)
IT Polyesters, preparation
(sulfo-containing, preparation of aqueous dispersions of, for
polyurethane binder compns.)
IT Polyesters, preparation
(sulfo-containing, graft, preparation of aqueous dispersions of, for
polyurethane binder compns.)
IT Polyesters, preparation
(**urethane** group-containing, preparation of aqueous dispersions of,
for **polyurethane** binder compns.)
IT 77-99-6DP, polyester **urethane** polyols, polymers with
polyisocyanates 85-42-7DP, Hexahydrophthalic anhydride,
polyester **urethane** polyols, polymers with
polyisocyanates 121-91-5DP, 1,3-Benzenedicarboxylic
acid, polyester **urethane** polyols, polymers with
polyisocyanates 126-30-7DP, Neopentyl glycol, polyester
urethane polyols, polymers with **polyisocyanates**
4098-71-9DP, polyester **urethane** polyols, polymers with
polyisocyanates 4767-03-7DP, polyester **urethane**
polyols, polymers with **polyisocyanates**
23501-81-7DP, Hexamethylene diisocyanate dimer,
polymers with polyester polyols 28574-90-5DP, polymers with
polyester polyols

(preparation of aqueous dispersions of, as binders)
 IT 26351-99-5P, Acrylic acid-Butyl acrylate-2-Hydroxyethyl
 methacrylate-Methyl methacrylate copolymer 153162-68-6P
 153354-09-7P 153354-10-0P
 (preparation of aqueous dispersions of, for polyurethane
 binders)

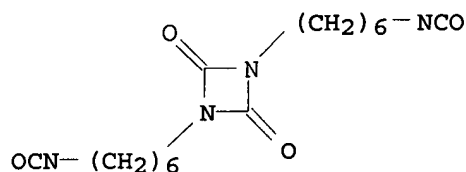
L50 ANSWER 19 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1994:32937 HCAPLUS
 DOCUMENT NUMBER: 120:32937
 TITLE: Modified polyureas for use in coatings
 INVENTOR(S): Muenzmay, Thomas; Hassel, Tillmann
 PATENT ASSIGNEE(S): Bayer A.-G., Germany
 SOURCE: Ger. Offen., 10 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4133572	A1	19930415	DE 1991-4133572	1991 1010
EP 538649	A1	19930428	EP 1992-116542	1992 0928
EP 538649	B1	19960612		
R: BE, DE, ES, FR, GB, IT, NL, SE				
ES 2088067	T3	19960801	ES 1992-116542	1992 0928
US 5284928	A	19940208	US 1992-956518	1992 1005
CA 2079980	AA	19930411	CA 1992-2079980	1992 1006
CA 2079980	C	20030211		
JP 06122750	A2	19940506	JP 1992-290963	1992 1006
JP 3107665	B2	20001113		
PRIORITY APPLN. INFO.:			DE 1991-4133572	A 1991 1010

AB Polyureas useful as binders for coatings contain anionic N-[(cyanoamino)carbonyl]urea groups and, optionally, terminal anionic cyanourea groups. Stirring hexanediol polycarbonate (OH number 56) 2240, a monofunctional ethylene oxide-rich polyether (OH number 26) 178, 3,5-bis(6-isocyanatohexyl)tetrahydro-1,3,5-oxadiazine-2,4,6-trione 336.4, HMDI 200.9, and IPDI 442.4 g at 80°, adding 94.8 g 1,4-butanediol, adding 6.5 kg acetone, adding 36.0 g ethylenediamine and 25.0 g hydrazine hydrate in 500 g H2O, stirring at 50°, adding a solution of cyanamide 33.6, Et3N 80.7, and acetone 300 g, stirring 60 min with removal of CO2, adding 8.6 kg H2O, and distilling acetone in vacuo

gave a dispersion (31.4% solids) showing DIN cup number 4 viscosity 12.5 s.

- IT 23501-81-7DP, polymers with polyols, **polyisocyanates** and diamines, reaction products with cyanamid, triethylamine salts (coatings, water-thinned, manufacture of)
- RN 23501-81-7 HCAPLUS
- CN 1,3-Diazetidione-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



- IC ICM C08G018-78
ICS C08G018-79; C08G018-32; C08G018-65; C09D175-02
- CC 42-7 (Coatings, Inks, and Related Products)
Section cross-reference(s): 37
- ST cyanamid adduct polyurea aq coating; **polyurethane** polyurea deriv aq coating; cyanobiuret polyurea deriv aq coating; polycarbonate polyurea **polyurethane** aq coating; oxadiazinetriene cyanoethyl copolymer aq coating
- IT **Urethane** polymers, uses
(polycarbonate-polyoxyalkylene-polyurea-, cyanobiuret group-containing, coatings, water-thinned, manufacture of)
- IT Polyureas
(polycarbonate-polyoxyalkylene-**polyurethane**-, cyanobiuret group-containing, coatings, water-thinned, manufacture of)
- IT Polyoxyalkylenes, uses
(polycarbonate-polyurea-**polyurethane**-, cyanobiuret group-containing, coatings, water-thinned, manufacture of)
- IT Polycarbonates, uses
(polyoxyalkylene-polyurea-**polyurethane**-, cyanobiuret group-containing, coatings, water-thinned, manufacture of)
- IT 107-15-3DP, 1,2-Ethanediamine, polymers with polyols, **polyisocyanates** and diamines, reaction products with cyanamid, triethylamine salts 110-63-4DP, 1,4-Butanediol, polymers with polyols, **polyisocyanates** and diamines, reaction products with cyanamid, triethylamine salts 302-01-2DP, Hydrazine, polymers with polyols, **polyisocyanates** and diamines, reaction products with cyanamid, triethylamine salts 420-04-2DP, Cyanamide, reaction products with polyureas, triethylamine salts 822-06-0DP, polymers with polyols, **polyisocyanates** and diamines, reaction products with cyanamid, triethylamine salts 4098-71-9DP, polymers with polyols, **polyisocyanates** and diamines, reaction products with cyanamid, triethylamine salts 23501-81-7DP, polymers with polyols, **polyisocyanates** and diamines, reaction products with cyanamid, triethylamine salts 25037-68-7DP, polymers with **polyisocyanates**, polyols and diamines, reaction products with cyanamide, triethylamine salts 50639-37-7DP, polymers with polyols, **polyisocyanates** and diamines, reaction products with cyanamid, triethylamine salts 152145-38-5DP, reaction products with cyanamide, triethylamine salts 152145-39-6DP, reaction products with cyanamide,

triethylamine salts
(coatings, water-thinned, manufacture of)

L50 ANSWER 20 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1994:32124 HCAPLUS
 DOCUMENT NUMBER: 120:32124
 TITLE: Free-flowing, thermoplastic, post-curable
 powdered polyurethanes, optionally expandable
 INVENTOR(S): Werner, Joachim; Meckel, Walter; Liman,
 Ulrich; Wegener, Dirk; Rasshofer, Werner;
 Rosthauser, James W.
 PATENT ASSIGNEE(S): Bayer A.-G., Germany
 SOURCE: Eur. Pat. Appl., 18 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 539802	A1	19930505	EP 1992-117604	1992 1015
R: BE, DE, ES, FR, GB, IT, NL, SE DE 4135475	A1	19930429	DE 1991-4135475	1991 1028
DE 4209709	A1	19930930	DE 1992-4209709	1992 0325
PRIORITY APPLN. INFO.:			DE 1991-4135475	A 1991 1028
			DE 1992-4209709	A 1992 0325

AB The title polyurethanes, useful in slush molding, are prepared by the reaction of emulsions of components bearing free NCO groups (or NCO-reactive groups) with components bearing an average of 2 NCO-reactive groups in the presence of a sep. prepared component bearing blocked NCO groups in an inert organic liquid carrier. Adipic acid-hexanediol-neopentyl glycol polyester (OH number 56) 68.2 and HMDI 19.7 parts were heated to 80°, mixed with 3.6 parts reaction product of 800 parts HMDI isocyanurate trimer and 543.9 parts Et 4-hydroxybenzoate, 2 parts Bu₂Sn dilaurate, 233 parts isooctane, and 7.8 parts 1,4-butanediol, stirred for 2 h at 90°, and cooled to give a free-flowing powder with particle size distribution 93.1% 100-315 µm and m.p. 160°. Heating a 1000-µm layer of this powder on glass at 200° for 20 min gave a film with tensile strength 27 MPa, elongation 751%, cut growth resistance 584 N/cm, and softening point 160°.

IT 151931-82-7
 (powder, preparation of thermoplastic, from emulsions)

RN 151931-82-7 HCAPLUS

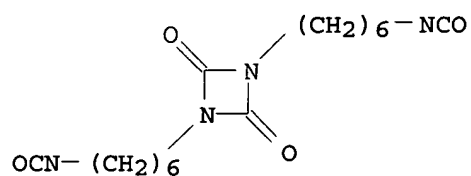
CN Hexanedioic acid, polymer with 1,3-bis(6-isocyanatohexyl)-1,3-

diazetidine-2,4-dione, 1,4-butanediol, 1,6-diisocyanatohexane,
2,2-dimethyl-1,3-propanediol and 1,6-hexanediol (9CI) (CA INDEX
NAME)

CM 1

CRN 23501-81-7

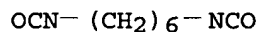
CMF C16 H24 N4 O4



CM 2

CRN 822-06-0

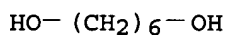
CMF C8 H12 N2 O2



CM 3

CRN 629-11-8

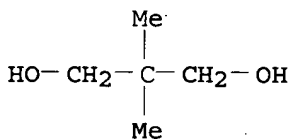
CMF C6 H14 O2



CM 4

CRN 126-30-7

CMF C5 H12 O2



CM 5

CRN 124-04-9

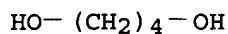
CMF C6 H10 O4



CM 6

CRN 110-63-4

CMF C4 H10 O2



IC ICM C08G018-08

ICS C08G018-10; C08G018-80; C08G018-79; C08J003-24

ICA C08L075-04

CC 37-3 (Plastics Manufacture and Processing)

IT 151931-81-6 151931-82-7 151931-83-8 151931-84-9

(powder, preparation of thermoplastic, from emulsions)

L50 ANSWER 21 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:604627 HCAPLUS

DOCUMENT NUMBER: 119:204627

TITLE: Polyisocyanate mixtures and their
preparation and use as crosslinking agents in
aqueous binder compositions

INVENTOR(S): Reiff, Helmut

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Ger. Offen., 9 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

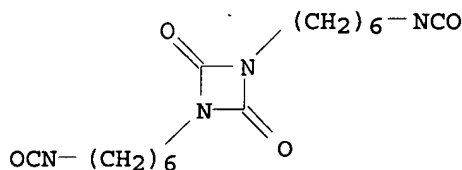
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4129953	A1	19930311	DE 1991-4129953	1991 0910
EP 531820	A1	19930317	EP 1992-114682	1992 0828
EP 531820 R: DE, FR, GB, IT	B1	19970709		
CA 2077633	AA	19930311	CA 1992-2077633	1992 0904
CA 2077633	C	20021119		
US 5258452	A	19931102	US 1992-940564	1992 0904
PRIORITY APPLN. INFO.:			DE 1991-4129953	A 1991 0910

AB A polyisocyanate composition containing (cyclo)aliphatic
isocyanate groups and having average NCO functionality

≥2.1 and a modifier containing ≥1 tertiary N and ≥1 isocyanate-reactive group are used to prepare a polyisocyanate mixture having an NCO functionality 2.3-4.3. The mixture is useful as a crosslinking composition, which forms stable aqueous emulsions. Reacting 50 g (2-hydroxyethyl)morpholine with 1 kg trimerized hexamethylene diisocyanate [mixture of tris(6-isocyanatohexyl) isocyanurate and higher homologs] having average NCO functionality 3.3 and adding 43.3 g Me₂SO₄ gave a product (NCO content 17.9%; quaternary N content 32.7 mequiv./100 g), which was mixed (25 g) with 75 g water to give an emulsion showing storage stability >1 day.

IT 23501-81-7DP, reaction products with amines
(preparation of emulsifiable, as crosslinking agents)
RN 23501-81-7 HCAPLUS
CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



IC ICM C08G018-78
ICS C08G018-79; C08G018-48; C09D175-04; C09J175-04
ICI C09D175-04, C09D133-04; C09D167-00, C09D167-08
CC 37-6 (Plastics Manufacture and Processing)
ST isocyanate mixt prepn emulsion crosslinker;
hexamethylene diisocyanate trimer deriv crosslinker;
hydroxyethylmorpholine polyisocyanate mixt emulsion
crosslinker; polyisocyanate mixt prepn emulsion
crosslinker; quaternary ammonium polyisocyanate emulsion
crosslinker; amine polyisocyanate emulsion crosslinker;
binder emulsion crosslinker polyisocyanate; adhesive
emulsion crosslinker polyisocyanate;
polyurethane emulsion crosslinker polyisocyanate
IT Emulsifying agents
(amine-polyisocyanate reaction products, for
polyisocyanate mixts. as crosslinking agents)
IT Adhesives
Binding materials
Coating materials
(crosslinking agents for, emulsifiable polyisocyanate
mixts. as)
IT Emulsions
(of polyisocyanate mixts., as crosslinking agents)
IT Crosslinking agents
(polyisocyanates, emulsifiable, for adhesives and
coatings)
IT Urethane polymers, preparation
(preparation and crosslinking of, emulsifiable
polyisocyanates for)
IT Quaternary ammonium compounds, preparation
(preparation of isocyanate group-containing, emulsifiable, as
crosslinking agents)
IT 77-78-1DP, Dimethylsulfate, quaternization products with amine
derivs. of polyisocyanates 103-76-4DP,

N-(2-Hydroxyethyl)piperazine, reaction products with **polyisocyanates** 108-19-0DP, Biuret, **isocyanate** derivs., reaction products with amines 622-40-2DP, N-(2-Hydroxyethyl)morpholine, reaction products with **polyisocyanates** 822-06-0DP, Hexamethylene **diisocyanate**, biuret and isocyanurate derivs., reaction products with amines 3040-44-6DP, N-(2-Hydroxyethyl)piperidine, reaction products with **polyisocyanates** 3779-63-3DP, Tris(6-**isocyanato**hexyl) isocyanurate, reaction products with amines 4035-89-6DP, N,N',N''-Tris(6-**isocyanato**hexyl)biuret, reaction products with amines 4098-71-9DP, Isophorone **diisocyanate**, trimers, reaction products with amines 9003-11-6DP, Ethylene oxide-propylene oxide copolymer, reaction products with amino derivs. of **polyisocyanates** 9038-95-3DP, Ethylene oxide-propylene oxide copolymer monobutyl ether, reaction products with amino derivs. of **polyisocyanates** 14037-23-1DP, reaction products with **polyisocyanates** 23501-81-7DP, reaction products with amines 25322-68-3DP, Polyethylene glycol, reaction products with amino derivs. of **polyisocyanates** 76996-65-1DP, reaction products with amino derivs. of **polyisocyanates** (preparation of emulsifiable, as crosslinking agents)

L50 ANSWER 22 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:86069 HCAPLUS

DOCUMENT NUMBER: 116:86069

TITLE: Syntheses and reactions of **urethanes** of cellobiose and cellulose-containing uretedione groups

AUTHOR(S): Meyer-Stork, L. Sebastian; Hoecker, Hartwig; Berndt, Heinz

CORPORATE SOURCE: RWTH Aachen, Aachen, 5100, Germany

SOURCE: Journal of Applied Polymer Science (1992), 44(6), 1043-9

CODEN: JAPNAB; ISSN: 0021-8995

DOCUMENT TYPE: Journal

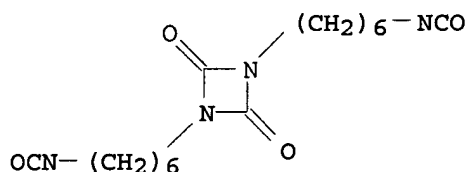
LANGUAGE: English

AB **Urethanes** of cellobiose and cellulose-containing uretedione groups are synthesized by the reaction of aliphatic and aromatic **diisocyanate** uretdiones with the saccharides. The syntheses are performed as a heterogeneous reaction in AcNMe₂ using dibutyltin dilaurate as catalyst, as well as a homogeneous reaction in AcNMe₂-LiCl. Thus, semisynthetic prepolymers are formed that offer the reactivity of (blocked) **isocyanate** groups. To demonstrate their reactivity, ring opening of the uretdiones is performed by the addition of a secondary amine to yield the corresponding ureas.

IT 23501-81-7DP, Hexamethylene **diisocyanate** dimer, reaction products with cellobiose or cellulose (preparation and structural characterization of)

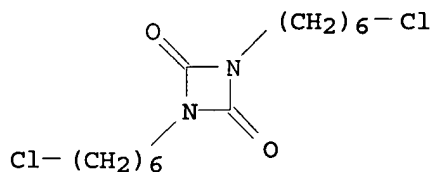
RN 23501-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA INDEX NAME)



CC 43-3 (Cellulose, Lignin, Paper, and Other Wood Products)
 Section cross-reference(s): 35
 ST **urethane** cellobiose cellulose uretedione
 IT 528-50-7DP, D-Cellobiose, reaction products with hexamethylene
diisocyanate dimer or TDI dimer 9004-34-6DP, Cellulose,
 reaction products with hexamethylene **diisocyanate** dimer
 or TDI dimer 23501-81-7DP, Hexamethylene
diisocyanate dimer, reaction products with cellobiose or
 cellulose 26747-90-0DP, TDI dimer, reaction products with
 cellobiose or cellulose
 (preparation and structural characterization of)

L50 ANSWER 23 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1988:529114 HCAPLUS
 DOCUMENT NUMBER: 109:129114
 TITLE: Synthesis and hydrolysis of (siloxylethyl)ureas
 AUTHOR(S): Vostokov, I. A.; Vasyaeva, L. V.
 CORPORATE SOURCE: Gos. Nauchno-Issled. Inst. Azotn. Prom.,
 Dzerzhinsk, USSR
 SOURCE: Zhurnal Obshchei Khimii (1987), 57(10),
 2329-33
 CODEN: ZOKHA4; ISSN: 0044-460X
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 109:129114
 AB 3,4-Cl₂C₆H₃NHCONRCH₂CH₂OSiMe₃ (R = H, CH₂CH₂OSiMe₃, SiMe₃) were
 prepared in 95-100% yields by treating 3,4-Cl₂C₆H₃NCO with
 RNHCH₂CH₂OSiMe₃. Hydrolysis of R₁NHCONRCH₂CH₂OSiMe₃ [R₁ =
 Cl(CH₂)₆, 3-ClC₆H₄, 3,4-Cl₂C₆H₃; R = H, CH₂CH₂OSiMe₃] gave 61-100%
 R₁NHCONRCH₂CH₂OH.
 IT 23336-46-1P
 (preparation of)
 RN 23336-46-1 HCAPLUS
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-chlorohexyl)- (9CI) (CA
 INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)
 ST addn **isocyanate** siloxyethylamine; siloxyethylurea; urea
 siloxyethyl phenyl; hydrolysis siloxyethylurea; hydroxyethylurea
 IT Addition reaction
 (of Ph **isocyanates** with siloxyethylamines,
 siloxyethylureas by)

IT 1025-36-1P 1785-02-0P 3420-84-6P 4459-90-9P 15145-34-3P
 16122-64-8P 23336-46-1P 23544-79-8P 69796-24-3P
 87919-35-5P 91933-84-5P 116422-02-7P 116422-03-8P
 116422-04-9P

(preparation of)

IT 20836-42-4
 (reaction of, with Ph **isocyanate**)

IT 17165-52-5
 (reaction of, with Ph **isocyanate** derivs.)

IT 111-42-2, Diethanolamine, reactions 5804-92-2 20836-40-2
 (reaction of, with dichlorophenyl **isocyanate**)

IT 102-36-3 103-71-9, Phenyl **isocyanate**, reactions
 2909-38-8 13654-91-6, 6-Chlorohexyl **isocyanate**
 (reaction of, with siloxyethylamines)

L50 ANSWER 24 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:511355 HCAPLUS

DOCUMENT NUMBER: 109:111355

TITLE: Analysis of chemical structures of
 isocyanurate-oxazolidone resins by infrared
 absorption spectroscopy

AUTHOR(S): Yokoyama, Takashi; Koyama, Toru; Kinjo,
 Noriyuki; Narahara, Toshikazu

CORPORATE SOURCE: Hitachi Res. Lab., Hitachi Ltd., Hitachi,
 319-12, Japan

SOURCE: Kobunshi Ronbunshu (1988), 45(6), 491-8
 CODEN: KBRBA3; ISSN: 0386-2186

DOCUMENT TYPE: Journal

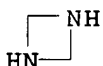
LANGUAGE: Japanese

AB Isocyanurate-oxazolidone resins were prepared from 2,4-TDI and
 2,2-bis[p-(2,3-epoxypropyloxy)phenyl]propane (I) using
 N-methylmorpholine as a catalyst. Model polymers containing
 isocyanurate, oxazolidone, and uretidindione rings were prepared
 from TDI, MDI, tri-Ph isocyanurate, and I in order to form
 calibration curves for IR spectra. Composition of hetero rings in the
 cured product varied with curing **temperature**, time, and compound
 ratio. **Isocyanate** groups changed mainly to isocyanurate
 rings with .apprx.20 mol% of the groups becoming oxazolidone
 rings. Product contents of uretidindione rings were <6 mol%.
 Reaction routes were analyzed from conversion ratios. Variations
 in the bending strength of the resins made from modified MDI and I
 are discussed in relation to hetero ring content.

IT 5663-08-1DP, 1,3-Diazetidine, derivs., polymers
 (preparation of, from **diisocyanates** and
 bis(epoxypropylphenyl)propane, hetero ring formation in, effect
 of curing conditions on)

RN 5663-08-1 HCAPLUS

CN 1,3-Diazetidine (9CI) (CA INDEX NAME)



CC 37-4 (Plastics Manufacture and Processing)

IT Ring closure and formation
 (in polymerization of **diisocyanates** and
 bis(epoxypropylphenyl)propane)

IT Polymerization

(of **diisocyanates** with bis[(epoxypropyl)phenyl]propane, mechanism of oxazolidone and isocyanurate and uretidindione ring formation in)

IT Chains, chemical
(structure of, of **diisocyanate**-bis(epoxypropylphenyl)propane copolymers, effect of curing conditions on)

IT 504-76-7DP, Oxazolidine, derivs., polymers **5663-08-1DP**, 1,3-Diazetidine, derivs., polymers
(preparation of, from **diisocyanates** and bis(epoxypropylphenyl)propane, hetero ring formation in, effect of curing conditions on)

L50 ANSWER 25 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:406994 HCAPLUS

DOCUMENT NUMBER: 109:6994

TITLE: Formation of a uretonimine in the production of heat-treated 4,4'-diphenylmethane **diisocyanate**

AUTHOR(S): Ivanov, M. G.; Golov, V. G.; Rogulev, V. A.; Mushkin, Yu. I.; Vodop'yanov, V. G.; Gerega, V. F.

CORPORATE SOURCE: USSR

SOURCE: Khimicheskaya Promyshlennost (Moscow, Russian Federation) (1988), (4), 208-10
CODEN: KPRMAW; ISSN: 0023-110X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

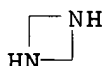
OTHER SOURCE(S): CASREACT 109:6994

AB In the thermal decarboxylation of MDI to give carbodiimide monomers containing NCO groups, a substituted uretonimine (1,3-diazacyclobutane derivative) was formed from reaction of the carbodiimide moiety with NCO groups of the MDI or the carbodiimide. The reaction was reversible at 120-180°. At 70° and lower, the reaction equilibrium shifted almost completely to the side of uretonimine formation. At 120° the equilibrium reaction mixture contained significant amts. of carbodiimide, resulting in a decrease in the content of trifunctional uretonimine and in a decrease of product functionality to 2. Kinetic data are given for the equilibrium reaction, and permit calcn. of the time necessary for achieving stable physicochem. properties of the product. Thus, 90-95% conversion of carbodiimide to uretonimine was achieved after 10-15 days at 20° or after 5-7 h at 70°.

IT **5663-08-1DP**, 1,3-Diazacyclobutane, derivs.
(formation of, in thermal decarboxylation of MDI to carbodiimide, kinetics and equilibrium of)

RN **5663-08-1** HCAPLUS

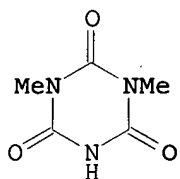
CN 1,3-Diazetidine (9CI) (CA INDEX NAME)



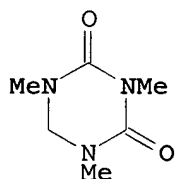
CC 35-2 (Chemistry of Synthetic High Polymers)

IT **5663-08-1DP**, 1,3-Diazacyclobutane, derivs.
(formation of, in thermal decarboxylation of MDI to carbodiimide, kinetics and equilibrium of)

L50 ANSWER 26 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1986:552526 HCAPLUS
 DOCUMENT NUMBER: 105:152526
 TITLE: Studies of methyl **isocyanate**
 chemistry in the Bhopal incident
 AUTHOR(S): D'Silva, Themistocles D. J.; Lopes, Anibal;
 Jones, Russell L.; Singhawangcha, Sureerat;
 Chan, John K.
 CORPORATE SOURCE: Res. Dev. Dep., Union Carbide Agric. Prod.
 Co., Inc., Research Triangle Park, NC, 27709,
 USA
 SOURCE: Journal of Organic Chemistry (1986), 51(20),
 3781-8
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:152526
 GI



II



III

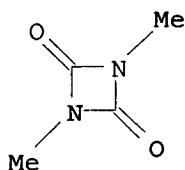
AB Following the MeNCO leak from Tank 610 at the Bhopal plant, the residual material from the tank was analyzed for its contents. Approx. 70% of the residue was comprised of 3 cyclic materials: MeNCO cyclotrimer, di-Me isocyanurate (I), and dihydrotrimethyltriazinedione (II). Minor quantities of methyl-substituted ureas, biurets, and amine hydrochlorides were also found. The composition of the residue was replicated very closely by the products obtained when a mixture of MeNCO (84.4%), CHCl₃ (12.0%), and water (3.6%) was heated at 225° under pressure in a stainless steel reactor. Exptl. results are consistent with the view that under these conditions MeNCO reacts initially with water to form 1,3-dimethylurea (III) and 1,3,5-trimethylbiuret (IV). At 100-225° these products decompose to reactive intermediates which further react exothermically to form the aforementioned cyclic materials, trimethylurea, and mono-, di-, and trimethylamine hydrochlorides. The decomposition of III and IV is facilitated by the presence of CHCl₃ and metals. Other expts. involving ¹³C-enriched CHCl₃ support the proposed mechanisms for formation of I and II.

IT 36909-44-1P

(preparation and detection of, Me **isocyanate** chemical and Bhopal incident in relation to)

RN 36909-44-1 HCAPLUS

CN 1,3-Diazetidione-2,4-dione, 1,3-dimethyl- (9CI) (CA INDEX NAME)



- CC 23-21 (Aliphatic Compounds)
- ST methyl **isocyanate** chem Bhopal; cyclotrimerization methyl **isocyanate**; triazinetrione methylated; isocyanurate dimethyl; triazinedione dihydrotrimethyl
- IT Trimerization
(cyclo-, of Me **isocyanate**, Bhopal incident in relation to)
- IT 75-44-5
(Me **isocyanate** reactions in presence of, Bhopal incident in relation to)
- IT 96-31-1
(detection and reactions of, Me **isocyanate** chemical and Bhopal incident in relation to)
- IT 506-59-2 593-51-1 593-81-7 632-22-4 7439-89-6, analysis
7440-02-0, analysis 7440-47-3, analysis
(detection of, Me **isocyanate** chemical and Bhopal incident in relation to)
- IT 67-66-3, uses and miscellaneous
(effect of, on Me **isocyanate** chemical)
- IT 6452-47-7
(preparation and Me **isocyanate** reactions in presence of, Bhopal incident in relation to)
- IT 13188-08-4P
(preparation and cyclocondensation of, Me **isocyanate** dimer from)
- IT 827-16-7P 6726-48-3P 36909-44-1P 41221-01-6P.
54070-65-4P
(preparation and detection of, Me **isocyanate** chemical and Bhopal incident in relation to)
- IT 632-14-4P 816-00-2P
(preparation, detection, and reaction of, Me **isocyanate** chemical and Bhopal incident in relation to)
- IT 31717-44-9
(reaction of, with Me **isocyanate**, Bhopal incident in relation to)
- IT 590-28-3
(reaction of, with Me **isocyanate**, dimethyltriazinetriene from)

L50 ANSWER 27 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:488088 HCAPLUS

DOCUMENT NUMBER: 99:88088

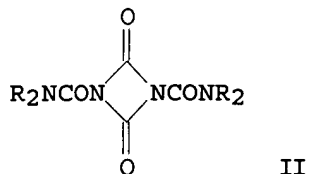
TITLE: Synthesis of carbamoyl **isocyanates**
by the exchange reaction of carbamoyl
chlorides with trimethylisocyanatosilane*
**

AUTHOR(S): Kozyukov, V. P.; Mironov, V. F.

CORPORATE SOURCE: Gos. Nauchno-Issled. Inst. Khim. Tekhnol.
Elementoorg. Soedin., Moscow, USSR

SOURCE: Zhurnal Obshchei Khimii (1983), 53(6), 1434-5
CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 99:88088
 GI

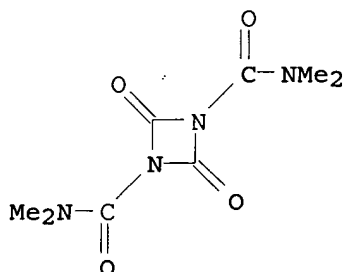


AB R2NC(O)NCO (I, R = Me, Et) are prepared in 70-90% yields by treatment of R2NCOCl with Me3SiNCO in the presence of SnCl4 3-5 h. I readily dimerize to give II which can be decomposed to the monomer at 200-300° and 2-3 mm pressure.

IT ***68661-66-5P 86790-60-5P
 (preparation and conversion to monomer)

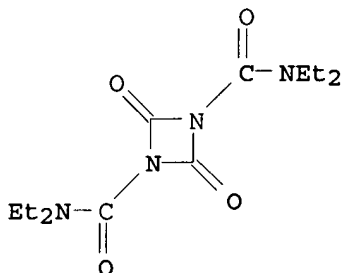
RN 68661-66-5 HCAPLUS

CN 1,3-Diazetidinedione-1,3-dicarboxamide, N,N,N',N'-tetramethyl-2,4-dioxo-
 (9CI) (CA INDEX NAME)



RN 86790-60-5 HCAPLUS

CN 1,3-Diazetidinedione-1,3-dicarboxamide, N,N,N',N'-tetraethyl-2,4-dioxo-
 (9CI) (CA INDEX NAME)



CC 28-4 (Heterocyclic Compounds (More Than One Hetero Atom))

ST diazetidinedione; isocyanate dimethylcarbamoyl
 cyclodimerization

IT Condensation reaction
 (of carbamoyl chlorides with trimethylsilyl isocyanate)

)
 IT Dimerization
 (cyclo-, of dialkylcarbamoyl **isocyanates**)
 IT **68661-66-5P 86790-60-5P**
 (preparation and conversion to monomer)
 IT 79-44-7 88-10-8
 (reaction of, with trimethylsilyl **isocyanate**)

L50 ANSWER 28 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1981:462141 HCAPLUS

DOCUMENT NUMBER: 95:62141

TITLE: Cycloaddition reactions between acyl (or thioacyl) **isocyanates** (or isothiocyanates) and **isocyanates** (or isothiocyanates)

AUTHOR(S): Ratton, Serge; Moyne, Jose; Longeray, Remi

CORPORATE SOURCE: Cent. Rech. Decines, Rhone-Poulenc Rech. Dev., Decines-Charpieu, 69150, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1981), (1-2, Pt. 2), 28-32

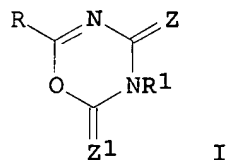
CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

OTHER SOURCE(S): CASREACT 95:62141

GI



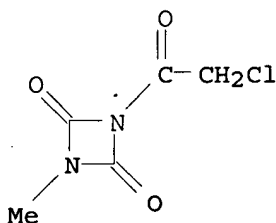
AB The reaction of RCONCZ [R = Ph, O₂NC₆H₄, 2,4-Me(Cl)C₆H₃OCH₂, 4,3,5-Cl(O₂N)₂C₆H₂, ClCH₂, PhOCH₂, Me₂N; Z = O, S] with R₁NCZ₁ (R₁ = Me, Et, Ph, 4-FC₆H₄; Z₁ = O, S) gave oxadiazines I. Thus, PhCONCO was added MeNCO in ether at 20°, and the mixture was stirred 120 h to give I (Z = Z₁ = O, R = Ph, R₁ = Me).

IT **78488-11-6P**

(preparation of)

RN 78488-11-6 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1-(chloroacetyl)-3-methyl- (9CI) (CA INDEX NAME)



CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 23, 25

ST oxadiazinedione; cycloaddn benzoyl **isocyanate**; methyl
isocyanate cycloaddn
IT Cycloaddition reaction
(of acyl **isocyanates** and carbamoyl isothiocyanate
derivative with organic **isocyanates** and isothiocyanates,
oxadiazines and thiadiazines from)
IT 4461-30-7 4461-31-8 4461-37-4 5843-49-2 41835-30-7
61831-98-9
(cycloaddn. reaction of, with Me **isocyanate**)
IT 103-71-9, reactions 109-90-0
(cycloaddn. reaction of, with benzoyl **isocyanate** and
carbamoyl isothiocyanate derivative)
IT 624-83-9
(cycloaddn. reaction of, with benzoyl **isocyanates** and
carbamoyl isothiocyanate derivative)
IT 4461-33-0
(cycloaddn. reaction of, with organic **isocyanates**)
IT 16011-79-3
(cycloaddn. reaction of, with organic **isocyanates** and
isothiocyanates)
IT 61831-87-6P 61831-88-7P 61831-89-8P 61831-90-1P
61831-91-2P 61831-92-3P 61831-94-5P 61831-95-6P
61831-96-7P 61831-97-8P 78488-10-5P 78488-11-6P
78488-12-7P 78488-13-8P 78488-14-9P 78488-15-0P
(preparation of)

L50 ANSWER 29 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:75625 HCAPLUS

DOCUMENT NUMBER: 92:75625

TITLE: Coordination properties of **isocyanates**

AUTHOR(S): Varentsova, N. V.; Gol'dshtein, I. P.;
Shufrina, R. R.; Shcherbakova, E. S.;
Tarakanov, O. G.; Gur'yanova, E. N.

CORPORATE SOURCE: Nauchno-Issled. Fiz.-Khim. Inst. im. Karpova,
Moscow, USSR

SOURCE: Zhurnal Obshchei Khimii (1979), 49(9), 2082-90
CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

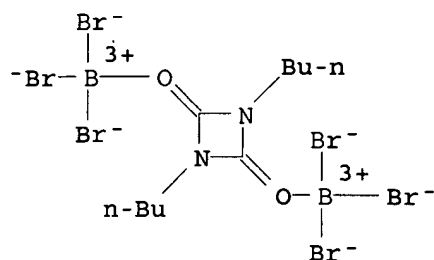
LANGUAGE: Russian

AB Calorimetric, cryoscopic and spectral data indicated that BuNCO
and PhNCO formed complexes with electron acceptors, e.g., SnCl₄,
CF₃CO₂H, BBr₃ and AlBr₃. The last 2 compds. also formed complexes
with cyclic dimers and trimers of the **isocyanates**. The
heats of formation of 2:1 complexes of AlBr₃ with BuNCO
and PhNCO were -28.3 and -17.2 kcal/mol, resp.; the values for the
corresponding BBr₃ complexes were -25.5 and -14.3 kcal/mol. The
isocyanates did not form complexes with tertiary amine
donors.

IT 72606-17-8P 72606-20-3P
(preparation of)

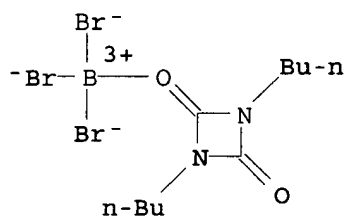
RN 72606-17-8 HCAPLUS

CN Boron, hexabromo[μ-(1,3-dibutyl-1,3-diazetidine-2,4-dione-
O:O')]di- (9CI) (CA INDEX NAME)



RN 72606-20-3 HCAPLUS

CN Boron, tribromo(1,3-dibutyl-1,3-diazetidine-2,4-dione-O)-, (T-4)-(9CI) (CA INDEX NAME)



CC 22-8 (Physical Organic Chemistry)

ST **isocyanate** complex electron acceptor; tin chloride complex **isocyanate**; aluminum bromide complex **isocyanate**; boron bromide complex **isocyanate**; fluoroacetic acid complex **isocyanate**

IT Ultraviolet and visible spectra

(of **isocyanate** complexes with aluminum bromide)

IT Infrared spectra

(of **isocyanate** complexes with boron bromide)

IT Molecular association

(of **isocyanates** with electron acceptors)

IT 110-86-1, reactions 121-44-8, reactions 280-57-9

(attempted complexation of, with **isocyanates**)

IT 7727-15-3 10294-33-4

(complexation of, with **isocyanates**)

IT 72576-88-6P 72576-89-7P 72576-90-0P 72606-14-5P

72606-15-6P 72606-16-7P 72606-17-8P 72606-18-9P

72606-19-0P 72606-20-3P 72606-21-4P 72606-22-5P

72606-23-6P 72606-24-7P 72627-57-7P

(preparation of)

L50 ANSWER 30 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1979:22234 HCAPLUS

DOCUMENT NUMBER: 90:22234

TITLE: Synthesis and properties of
(N,N-dimethyl)dichloromethaniminium
chlorosulfate

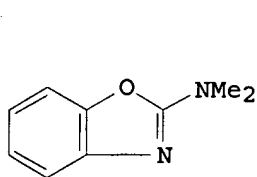
AUTHOR(S): Kukhar, V. P.; Pasternak, V. I.; Shevchenko,
M. V.

CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR

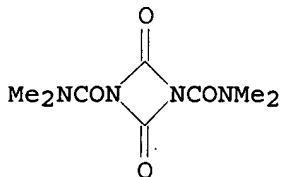
SOURCE: Zhurnal Organicheskoi Khimii (1978), 14(9),
1841-6

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 90:22234
 GI



VI



VII

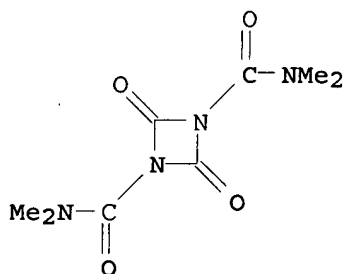
AB $\text{Cl}_2\text{C:NMe}_2 + \text{X}^-$ [I; X = Cl (II)] reacted with Me_2SO_4 to give I [X = ClSO_3 (III)] via the intermediate I [X = MeOSO_3 (IV)]. III was also prepared directly from II in 81% yield by treatment with ClSO_3H , and along with I (X = ClSO_3SO_3) by treatment with SO_3 . Analogously, $\text{Z:NMe}_2 + \text{X}^-$ (V; Z = CH_2 , ClCH ; X = Cl) reacted with SO_3 to give 85-96% V (Z = same; X = ClSO_3 , ClSO_3SO_3). Pyrolysis of III gave 80% Me_2NCOCl , SO_2 and Cl_2 . III and IV cyclized with o- $\text{H}_2\text{NC}_6\text{H}_4\text{OH}$ to give benzoxazole VI. III reacted with p- $\text{ClC}_6\text{H}_4\text{SO}_2\text{NCl}_2$ to give 41% p- $\text{ClC}_6\text{H}_4\text{SO}_2\text{N:CClNMe}_2$, and with $\text{Cl}_2\text{NCO}_2\text{Et}$ to give 83% Me_2NCONCO , which underwent partial cyclodimerization to VI on distillation and reacted with PhNH_2 to give $\text{Me}_2\text{NCONHCONHPh}$.

IT 68661-66-5P

(preparation of)

RN 68661-66-5 HCAPLUS

CN 1,3-Diazetidone-1,3-dicarboxamide, N,N,N',N'-tetramethyl-2,4-dioxo-
 (9CI) (CA INDEX NAME)



CC 23-4 (Aliphatic Compounds)

Section cross-reference(s): 28

IT 62-53-3, reactions

(addition reaction of, with dimethylcarbamoyl isocyanate)

IT 2617-87-0P 13858-89-4P 34520-13-3P 68661-60-9P 68661-62-1P

68661-66-5P 68661-67-6P

(preparation of)

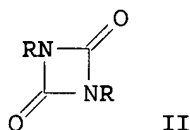
L50 ANSWER 31 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:615264 HCAPLUS

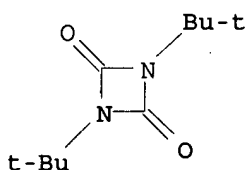
DOCUMENT NUMBER: 89:215264

TITLE: Synthesis of 1,3-dialkyldiazetidinediones from

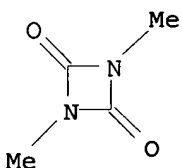
N,N'-dialkylaminocarbonylcarbamic chlorides
 (2,4-dialkylallophanoyl chlorides)
 AUTHOR(S): White, Dabney K.; Greene, Frederick D.
 CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol.,
 Cambridge, MA, USA
 SOURCE: Journal of Organic Chemistry (1978), 43(23),
 4530-2
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 89:215264
 GI



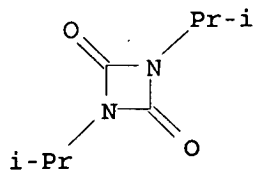
AB Hydrolyzing the title carbamoyl chlorides, RN:CClNRCOCl (R =
 CHMe₂, cyclohexyl, CMe₃) in acetone-water gave 60-80% RNHCONRCOCl
 (I). Treating I with 1,4-diazabicyclo[2.2.2]octane in ether gave
 55-84% 1,3-dialkyl-2,4-diazetidinediones II (R = CHMe₂,
 cyclohexyl, CMe₃, Me). Use of NaH or KOtMe₃ to promote ring
 closure of I gave mixts. of products.
 IT 30885-14-4P 36909-44-1P 67463-80-3P
 (preparation of)
 RN 30885-14-4 HCAPLUS
 CN 1,3-Diazetidinedione-2,4-dione, 1,3-bis(1,1-dimethylethyl)- (9CI) (CA
 INDEX NAME)



RN 36909-44-1 HCAPLUS
 CN 1,3-Diazetidinedione-2,4-dione, 1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 67463-80-3 HCAPLUS
 CN 1,3-Diazetidinedione-2,4-dione, 1,3-bis(1-methylethyl)- (9CI) (CA
 INDEX NAME)

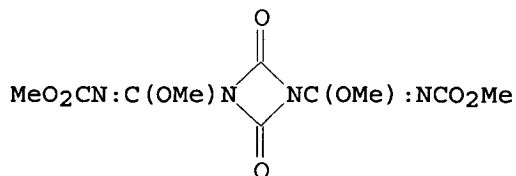


CC 28-4 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 15234-14-7P 30885-14-4P 36909-44-1P
 51170-55-9P 67463-80-3P 67463-81-4P
 (preparation of)
 IT 75-65-0, reactions
 (reaction of, with iso-Pr isocyanate)

L50 ANSWER 32 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1978:6583 HCAPLUS
 DOCUMENT NUMBER: 88:6583
 TITLE: Alkoxycarbonylisourea isocyanates
 INVENTOR(S): Fuchs, Julius Jakob
 PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA
 SOURCE: U.S., 5 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4045473	A	19770830	US 1975-603651	1975 0811
US 4075201	A	19780221	US 1977-776258	1977 0310
PRIORITY APPLN. INFO.:			US 1975-603651	A3 1975 0811

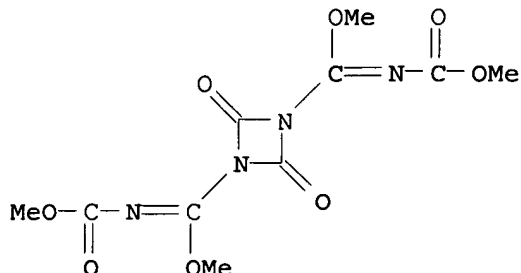
GI



AB MeO₂CN:C(OMe)NH₂, prepared from MeOC(NH₂):NH and MeO₂CCl, was treated with Cl₂CO to give the diazotidine biscarbamate I via MeO₂CN:C(OMe)NCO. I was treated with cyclohexylamine to give RNHCONHC(OMe):NCO₂Me (II, R = cyclohexyl). II (R = p-ClC₆H₄) was similarly prepared II were herbicidal (no data).
 IT 64836-49-3P

(preparation and reaction with amines)

RN 64836-49-3 HCAPLUS

CN 1,3-Diazetidine-1,3-dicarboximidic acid, N,N'-bis(methoxycarbonyl)-
2,4-dioxo-, dimethyl ester (9CI) (CA INDEX NAME)

IC C07C127-26

INCL 260482000C

CC 25-28 (Noncondensed Aromatic Compounds)

Section cross-reference(s): 5

ST allophanimidate prepn herbicide; diazetidine biscarbamate;
isocyanate alkoxy carbonyl isourea

IT 64836-49-3P

(preparation and reaction with amines)

L50 ANSWER 33 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:423111 HCAPLUS

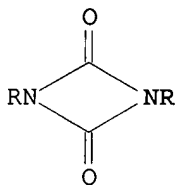
DOCUMENT NUMBER: 87:23111

TITLE: 1,3-Dialkyldiazetidin-2,4-diones. Structure
and molecular spectraAUTHOR(S): Kuhn, Norbert; Schwarz, Wolfgang; Schmidt,
ArminCORPORATE SOURCE: Inst. Anorg. Chem., Univ. Stuttgart,
Stuttgart, Fed. Rep. Ger.SOURCE: Chemische Berichte (1977), 110(3), 1130-9
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



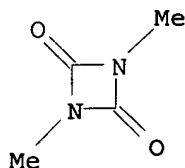
I

AB Diazetidinediones I (R = Me, Et) were prepared by cyclizing
dimerization of the corresponding RNCO (R = Me, Et) with SbCl₅.
The vibrational spectra of I (R = Me, Et) were discussed. The
crystal and mol. structure of I (R = Me) were determined, as well as ¹H
NMR data for I (R = Me, Et).

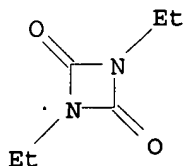
IT 36909-44-1P

(preparation and crystal and mol. structure and spectra of)

RN 36909-44-1 HCAPLUS
CN 1,3-Diazetidine-2,4-dione, 1,3-dimethyl- (9CI) (CA INDEX NAME)

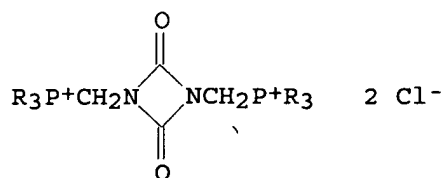


IT 23336-34-7P
(preparation and spectra of)
RN 23336-34-7 HCAPLUS
CN 1,3-Diazetidine-2,4-dione, 1,3-diethyl- (9CI) (CA INDEX NAME)



CC 28-4 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 22, 75
ST alkyl **isocyanate** cyclodimerization; diazetidinedione
crystal mol structure; vibrational spectra diazetidinedione; NMR
diazetidinedione
IT 7647-18-9
(cyclodimerization of alkyl **isocyanates** in presence
of)
IT 36909-44-1P
(preparation and crystal and mol. structure and spectra of)
IT 23336-34-7P
(preparation and spectra of)

L50 ANSWER 34 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:190109 HCAPLUS
DOCUMENT NUMBER: 86:190109
TITLE: Trialkyl- and triaryl(isocyanatomethyl
)chlorophosphoranes
AUTHOR(S): Kozhushko, B. N.; Gumenyuk, A. V.; Paliichuk,
Yu. A.; Shokol, V. A.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Zhurnal Obshchei Khimii (1977), 47(2), 333-9
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



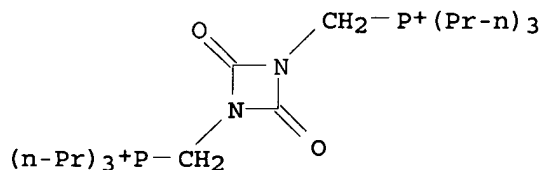
II

AB $\text{R}_3\text{P}^+\text{CH}_2\text{NCO Cl}^-$ (I; R = Ph, p-MeOC₆H₄, p-MeC₆H₄) and II (R = Pr, octyl, decyl) were prepared in 84-96% yields by treating R₃P with ClCH₂NCO in ether at 0-10°. I dimerized in the presence of Pr₃P in CHCl₃ to give the corresponding aryl dimers II. Treating I or II with R₁OH gave 12 $\text{R}_3\text{P}^+\text{CH}_2\text{NHCO}_2\text{R}_1 \text{ Cl}^-$ (R₁ = Me, Et, Pr, Me₂CH, Bu, Ph, α-naphthyl) in 50-92% yield.

IT 62779-07-1P 62779-08-2P 62779-09-3P
(preparation and reaction with alcs.)

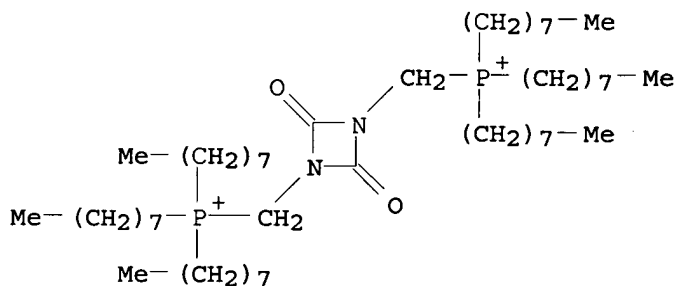
RN 62779-07-1 HCAPLUS

CN Phosphonium, [(2,4-dioxo-1,3-diazetidene-1,3-diyl)bis(methylene)]bis[tripropyl-, dichloride (9CI) (CA INDEX NAME)

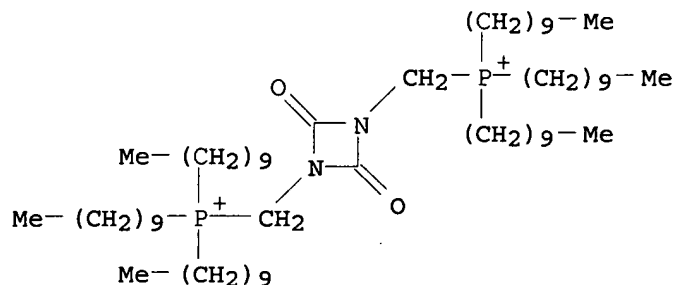
● 2 Cl⁻

RN 62779-08-2 HCAPLUS

CN Phosphonium, [(2,4-dioxo-1,3-diazetidene-1,3-diyl)bis(methylene)]bis[trioctyl-, dichloride (9CI) (CA INDEX NAME)

● 2 Cl⁻

RN 62779-09-3 HCAPLUS
 CN Phosphonium, [(2,4-dioxo-1,3-diazetidine-1,3-diyl)bis(methylene)]bis[tris(decyl)-, dichloride (9CI) (CA INDEX NAME)



● 2 Cl⁻

CC 29-7 (Organometallic and Organometalloidal Compounds)
 ST phosphonium **isocyanatomethyl** alkyl aryl; phosphorane
isocyanatomethyl alkyl aryl; **isocyanate**
 phosphorane
 IT Alcohols, reactions
 (reaction of, with **isocyanatomethylphosphonium**
 chlorides)
 IT 21955-22-6P 62779-07-1P 62779-08-2P
 62779-09-3P 62779-10-6P 62779-11-7P 62779-12-8P
 62779-13-9P 62779-14-0P
 (preparation and reaction with alcs.)
 IT 603-35-0, reactions 855-38-9 1038-95-5 2234-97-1 4731-53-7
 17621-07-7
 (reaction of, with chloromethyl **isocyanate**)
 IT 64-17-5, reactions 67-56-1, reactions 67-63-0, reactions
 71-23-8, reactions 71-36-3, reactions 108-95-2, reactions
 1321-67-1
 (reaction of, with **isocyanatomethylphosphonium**
 chlorides)

L50 ANSWER 35 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:509180 HCAPLUS

DOCUMENT NUMBER: 85:109180

TITLE: Thermostable polymers obtained by
 heating an aromatic imine with a
polyisocyanate

INVENTOR(S): Balme, Maurice; Gruffaz, Max; Rollet, Bernard
 PATENT ASSIGNEE(S): Societe des usines chimiques de Rhone-Poulenc,
 Fr.

SOURCE: Fr. Demande, 20 pp.
 CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

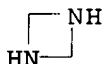
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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 FR 2279780 A1 19760220 FR 1974-25386 1974
 0722
 FR 2279780 B1 19770325
 PRIORITY APPLN. INFO.: FR 1974-25386 A 1974
 0722

AB Polymers resistant to heating at $\leq 180^\circ$
 were prepared by treating 4,4'-diisocyanatodiphenylmethane
 (I) with a benzylideneaminobenzene and optionally a bismaleimide.
 A mixture of 75.8 g 4,4'-bis(benzylideneamino)methane and 50 g I was
 heated 135 min at 260° and 5-8 g CO₂ was evolved.
 A polyimine diisocyanate was obtained which softened at
 $176-80^\circ$ and 50 g of this polymer was treated with 150 g
 4,4'-bis(maleimido)diphenylmethane and heated 30 min at
 $165-70^\circ$ to give a polymer softening at $148-50^\circ$ which
 was molded in 1 hr at 250° and 200 bars to give a product
 with initial flexural strength 5.1 kg/mm² and flexural modulus 232
 kg/mm² which changed to 6.8, 6.5, and 6.7 kg/mm² and 266, 257, and
 226 kg/mm² for strength and modulus resp., after 1160, 2230, and
 3250 hr at 250° .
 IT 5663-08-1DP, 1,3-Diazetidine, derivs., polymers
 (heat-resistant)
 RN 5663-08-1 HCAPLUS
 CN 1,3-Diazetidine (9CI) (CA INDEX NAME)



IC C08G033-02
 CC 35-3 (Synthetic High Polymers)
 ST benzylideneamino arom isocyanate polymer; polyimine
 polyisocyanate prepn; heat resistant polyimine
 isocyanate
 IT Heat-resistant materials
 (aromatic imine-aromatic diisocyanate polymers)
 IT 5663-08-1DP, 1,3-Diazetidine, derivs., polymers
 55719-52-3 55719-53-4 55753-37-2
 (heat-resistant)

L50 ANSWER 36 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1976:91789 HCAPLUS
 DOCUMENT NUMBER: 84:91789
 TITLE: Polyaddition products containing uretedione
 groups
 INVENTOR(S): Mueller, Hanns P.; Wagner, Kuno; Mueller,
 Richard
 PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 36 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO. -----	KIND ----	DATE -----	APPLICATION NO. -----	DATE
DE 2420475	A1	19751106	DE 1974-2420475	1974 0427
DE 2420475	C2	19871203		
AU 7579786	A1	19761007	AU 1975-79786	1975 0403
CA 1084196	A1	19800819	CA 1975-223960	1975 0407
US 4044171	A	19770823	US 1975-569112	1975 0417
DK 7501793	A	19751028	DK 1975-1793	1975 0424
SE 7504773	A	19751028	SE 1975-4773	1975 0424
NL 7504862	A	19751029	NL 1975-4862	1975 0424
GB 1492102	A	19771116	GB 1975-17005	1975 0424
BE 828385	A1	19751027	BE 1975-155767	1975 0425
FR 2268840	A1	19751121	FR 1975-13112	1975 0425
FR 2268840	B1	19790330		
BR 7502548	A	19760303	BR 1975-3232	1975 0425
ES 436992	A1	19770116	ES 1975-436992	1975 0425
AT 7503187	A	19770515	AT 1975-3187	1975 0425
AT 341221	B	19780125		
CH 616169	A	19800314	CH 1975-5330	1975 0425
JP 50149793	A2	19751201	JP 1975-50261	1975 0426
JP 57046447	B4	19821004		
PRIORITY APPLN. INFO.:			DE 1974-2420475	A 1974 0427

AB Dimerization of diisocyanates in the presence of Bu₃P or dibutyltin dilaurate (I) and polymerization with diols gave uretedione group-containing polyurethanes useful as hardeners for powdered

polyester-based coating materials. Thus, a mixture of 2,4-tolylene diisocyanate 313.2, MeOCH₂CH₂OAc 975, PhMe 325, and Bu₃P 7.2 parts was stirred for 3.5 hr at 10-15°, treated with 10% S solution in PhMe 22.8 hexamethylene diisocyanate 33.6, benzoyl chloride 0.3, I 0.4, and 2-ethyl-1,3-hexanediol 182 parts, and stirred for 4 hr at 100° to give polyurethane (II) [58407-19-5] with 140-55° m.p., 3826 mol. weight and 11.35% latent NCO content. A mixture of polyester 100, II 34, TiO₂, and butyl acrylate-2-ethylhexyl acrylate copolymer [58247-84-0] 10 parts was melted, solidified, pulverized sprayed on a metal sheet at 20-100 kV, and hardened at 160-220° to give a coating with 9 mm Erichsen deep-drawing elasticity (DIN 53 156), 37% elongation as determined with conical mandrel (ASTM D 522-41), and 3H pencil hardness (DIN 46 450).

IT 58247-83-9

(coatings, containing polyesters, electrostatic powder)

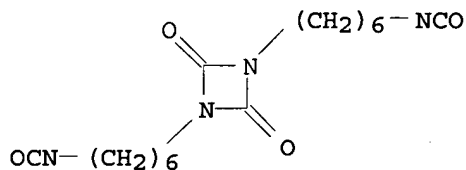
RN 58247-83-9 HCAPLUS

CN 1,3-Diazetidone-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with 1,2-ethanediol and 2-ethyl-1,3-hexanediol (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

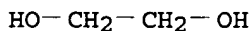
CMF C16 H24 N4 O4



CM 2

CRN 107-21-1

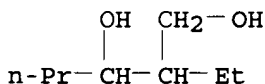
CMF C2 H6 O2



CM 3

CRN 94-96-2

CMF C8 H18 O2



IT 58247-81-7 58247-82-8

(hardeners, for polyesters)

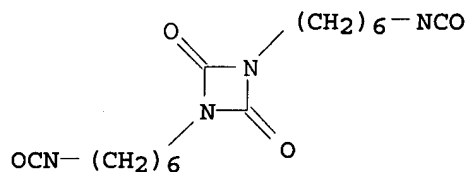
RN 58247-81-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, polymer with 1,4-butanediol (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

CMF C16 H24 N4 O4



CM 2

CRN 110-63-4

CMF C4 H10 O2

HO-(CH₂)₄-OH

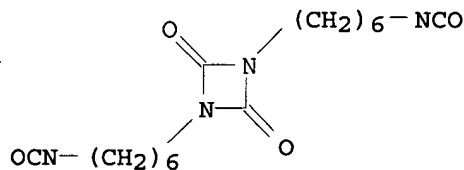
RN 58247-82-8 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 23501-81-7

CMF C16 H24 N4 O4



IC C08G

CC 42-9 (Coatings, Inks, and Related Products)

IT 31532-63-5 58247-83-9 58407-19-5

(coatings, containing polyesters, electrostatic powder)

IT 58247-81-7 58247-82-8 58342-52-2 58383-47-4

58383-48-5 58383-49-6 58383-50-9 58383-51-0 58383-52-1

58383-53-2 58383-54-3 58383-55-4 58383-56-5 58407-20-8

(hardeners, for polyesters)

L50 ANSWER 37 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

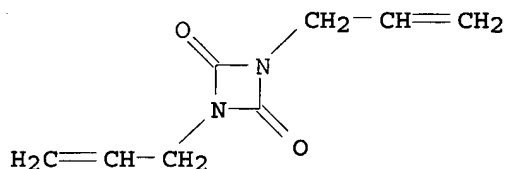
ACCESSION NUMBER: 1975:514346 HCAPLUS

DOCUMENT NUMBER: 83:114346

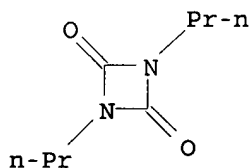
TITLE: Triallyl isocyanurate and products from the organomagnesium compounds reactions

AUTHOR(S): Etienne, Andre; Lonchambon, Georges;

Giraudeau, Pierre; Jaubert, Bernard
 CORPORATE SOURCE: Lab. Chim. Ind., Conservatoire Natl. Arts
 Metiers, Paris, Fr.
 SOURCE: Comptes Rendus des Seances de l'Academie des
 Sciences, Serie C: Sciences Chimiques (1975),
 280(15), 995-8
 CODEN: CHDCAQ; ISSN: 0567-6541
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 OTHER SOURCE(S): CASREACT 83:114346
 GI For diagram(s), see printed CA Issue.
 AB Triallyl isocyanurate (I) was prepared by trimerizing $\text{CH}_2\text{:CHCH}_2\text{NCO}$
 in $\text{ClCH}_2\text{CH}_2\text{Cl}$ in the presence of Bu_3P . I hydrolyzed in base to
 1,3,5-triallylbiuret. Reaction of I with organomagnesium halides
 gave the triazinols II ($\text{R} = \text{Me}, \text{Et}, \text{CH}_2\text{Ph}, \text{Ph}, \text{C}_6\text{H}_4\text{Cl-4}$). II
 dehydrated on distillation under N to give III ($\text{X} = \text{CH}_2, \text{CHMe}, \text{CHPh}$),
 which formed salts with acids.
 IT 23336-35-8P 56601-12-8P
 (preparation of)
 RN 23336-35-8 HCAPLUS
 CN 1,3-Diazetidine-2,4-dione, 1,3-di-2-propenyl- (9CI) (CA INDEX
 NAME)



RN 56601-12-8 HCAPLUS
 CN 1,3-Diazetidine-2,4-dione, 1,3-dipropyl- (9CI) (CA INDEX NAME)



CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 4015-16-1P 23336-35-8P 36020-44-7P 56601-12-8P
 56601-16-2P 56601-17-3P 56601-18-4P 56601-19-5P
 56601-20-8P 56601-22-0P 56601-23-1P 56601-25-3P
 56601-27-5P 56601-29-7P 56601-30-0P
 (preparation of)
 IT 998-40-3
 (trimerization of allyl isocyanate in presence of)

L50 ANSWER 38 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1972:572104 HCAPLUS
 DOCUMENT NUMBER: 77:172104
 TITLE: Phosphorothio(isocyanatidic)
 bis(dimethylamide) and bis(diethylamide)
 AUTHOR(S): Boden, Gisela; Grosskreutz, Werner; Kessler,
 Gudrun; Scheler, Hermann

CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden,
Ger. Dem. Rep.

SOURCE: Zeitschrift fuer Chemie (1972), 12(8), 299
CODEN: ZECEAL; ISSN: 0044-2402

DOCUMENT TYPE: Journal

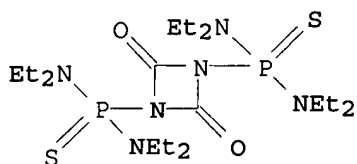
LANGUAGE: German

AB The reaction of (R₂N)₂P(S)Cl with AgOCN gave (R₂N)₂P(S) NCO [R =
Me (I) or Et (II)]. I was also prepared by reaction of
(Me₂N)₂P(S)NH₂ (III) with COCl₂. Reaction of I with NH₃(g) gave
(Me₂N)₂P(S)NHCONH₂. Reaction of II with 2,4,5-Cl₃C₆H₂NH₂ gave
(Et₂N)₂P(S)NHCONHC₆H₂Cl₃-2,4,5. Hydrolysis of I and II gave III
and (Et₂N)₂P(S)NH₂, resp. Reaction of dimeric (Et₂N)₂PNCO (IV)
with S gave [(Et₂N)₂P(S)NCO]₂ (V) of uretedione structure. The
reaction of dimeric IV with SPCL₃ gave V, Et₂NPCL₂,
Et₂NP(S)(NCO)₂, and II.

IT **38590-06-6P**
 (preparation of)

RN 38590-06-6 HCAPLUS

CN Phosphonothioic diamide, P,P'-(2,4-dioxo-1,3-diazetidine-1,3-
diyl)bis[N,N,N',N'-tetraethyl- (9CI) (CA INDEX NAME)



CC 78-8 (Inorganic Chemicals and Reactions)

ST **phosphorothioisocyanatidic** diamide;
 isocyanatothiophosphoric diamide; thioisocyanotophosphoric
 diamide; ureidothiophosphoric diamide; amide thiophosphoryl

IT 1069-08-5P 5022-58-2P 38590-03-3P 38590-05-5P
 38590-06-6P 38590-08-8P 38590-10-2P
 (preparation of)

L50 ANSWER 39 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1971:540742 HCAPLUS

DOCUMENT NUMBER: 75:140742

TITLE: Di-tert-butyluretidinedione

AUTHOR(S): Stowell, John C.; Greene, Frederick D.;
Bergmark, William R.

CORPORATE SOURCE: Dep. Chem., Louisiana State Univ., New
Orleans, LA, USA

SOURCE: Journal of Organic Chemistry (1971), 36(20),
3056-7
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

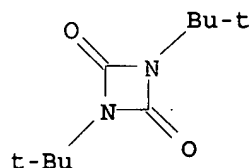
LANGUAGE: English

AB Reaction of Me₃CNHCONHCMe₃ with pyridine-phosgene affords
di-tert-butyluretidinedione and di-tert-butylcarbodiimide. Both
photolysis and thermolysis (200°) of the uretidinedione
afford Me₃CNCO.

IT **30885-14-4P**
 (preparation of)

RN 30885-14-4 HCAPLUS

CN 1,3-Diazetidone-2,4-dione, 1,3-bis(1,1-dimethylethyl)- (9CI) (CA
INDEX NAME)

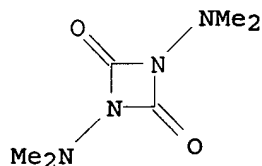


CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
 ST uretidinedione butyl; **isocyanate** butyl
 IT **30885-14-4P**
 (preparation of)

L50 ANSWER 40 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1971:13211 HCAPLUS
 DOCUMENT NUMBER: 74:13211
 TITLE: Silicon-nitrogen cleavage reactions in
 N,N-dimethyl-N',N'-dimethyl-N',N'-
 bis(trimethylsilyl)hydrazine
 AUTHOR(S): Glemser, Oskar; Kluever, Horst
 CORPORATE SOURCE: Anorg.-Chem. Inst., Univ. Goettingen,
 Goettingen, Fed. Rep. Ger.
 SOURCE: Chemische Berichte (1970), 103(11), 3661-6
 CODEN: CHBEAM; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: German

AB Treatment of $\text{Me}_2\text{NN}(\text{SiMe}_3)_2$ (I) with COF_2 in petroleum ether at -30° to 0° or with POF_3 in MeCN at -20° , yielded Me_3SiF (II) and bis(dimethylaminoisocyanate) or $\text{Me}_2\text{NN}[\text{P}(\text{O})\text{F}_2]\text{SiMe}_3$, resp. Reaction of I with $\text{P}_2\text{O}_3\text{F}_4$ containing $\text{HOP}(\text{O})\text{F}_2$ in Et_2O at 0° gave $\text{Me}_2\text{NNHP}(\text{O})\text{F}_2$ and $\text{Me}_3\text{SiOP}(\text{O})\text{F}_2$. Heating I and POCl_3 at 80° yielded $\text{Me}_2\text{NN}[\text{P}(\text{O})\text{Cl}_2]_2$ and Me_3SiCl . Reaction of I and PSF_3 in MeCN at 30° in an autoclave gave $\text{Me}_2\text{NN}[\text{P}(\text{S})\text{F}_2]\text{SiMe}_3$ and II.

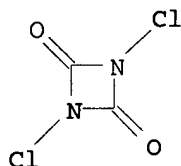
IT **29938-12-3P**
 (preparation of)
 RN 29938-12-3 HCAPLUS
 CN 1,3-Diazetidinedione-2,4-dione, 1,3-bis(dimethylamino)- (9CI) (CA
 INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)
 IT **29938-12-3P** 29938-13-4P 29938-14-5P 29938-15-6P
 30041-94-2P
 (preparation of)

L50 ANSWER 41 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1970:100564 HCAPLUS
 DOCUMENT NUMBER: 72:100564
 TITLE: Chemistry of **chloroisocyanate**. III.

1,3-Dichlorouretidinedione, a new
chloroisocyanate dimer
 AUTHOR(S): Gottardi, W.; Henn, D.
 CORPORATE SOURCE: Inst. Anorg. Anal. Chem., Univ. Innsbruck,
 Innsbruck, Austria
 SOURCE: Monatsh. Chem. (1970), 101(1), 264-74
 CODEN: MOCHAP
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI For diagram(s), see printed CA Issue.
 AB The phys. and chemical properties of 1,3-dichlorouretidine-2,4-dione
 (I) (ibid., 1969) are described. Upon **heating**, I gave,
 depending on the conditions, ClNCO, Cl₂NCONCO, or
 1,3,5-trichloro-2,4,6-trioxohexahydro-s-triazine. The reaction of
 I with EtOH gave ClNHCONHCO₂Et and H₂NCONHCO₂Et.
 IT 24604-62-4P
 (preparation of)
 RN 24604-62-4 HCAPLUS
 CN 1,3-Diazetidione-2,4-dione, 1,3-dichloro- (9CI) (CA INDEX NAME)



CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
 ST chloro uretidinone; uretidinone chloro; **isocyanate**
 chloro dimer; dimer **isocyanate** chloro; uretidinediones
 IT 14628-80-9P 24604-62-4P 26231-93-6P 26231-94-7P
 26231-96-9P
 (preparation of)

L50 ANSWER 42 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:67449 HCAPLUS

DOCUMENT NUMBER: 72:67449

TITLE: Chemistry of chlorine **isocyanate**.
 1. Polymerization, thermal behavior, and
 photolysis

AUTHOR(S): Gottardi, W.; Henn, D.

CORPORATE SOURCE: Inst. Anorg. Anal. Chem., Univ. Innsbruck,
 Innsbruck, Austria

SOURCE: Monatsh. Chem. (1969), 100(6), 1860-7
 CODEN: MOCHAP

DOCUMENT TYPE: Journal

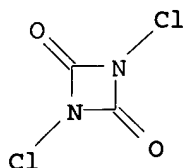
LANGUAGE: German

AB Liquid ClNCO polymerized on standing at 50° to
 1,3-dichlorouretidinedione, trimers, and low polymers. ClNCO(g)
 was stable in the dark at normal pressures and **temps.**,
 and at reduced pressures and elevated **temps.** ClNCO was
 extremely sensitive to photolysis, decomposing to Cl₂CO, N, CO, and
 ClCONCO. The possibility of storing ClNCO and using it
 synthetically were discussed.

IT 24604-62-4P
 (preparation of)

RN 24604-62-4 HCAPLUS

CN 1,3-Diazetidione-2,4-dione, 1,3-dichloro- (9CI) (CA INDEX NAME)



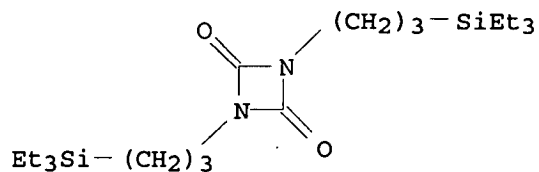
CC 35 (Synthetic High Polymers)
 ST chlorine **isocyanate** thermolysis photolysis;
isocyanate chlorine thermolysis photolysis; thermolysis
 photolysis chlorine **isocyanate**; photolysis thermolysis
 chlorine **isocyanate**
 IT Ring closure
 (in oligomerization, of chlorine **isocyanate**)
 IT Photolysis
 (of chlorine **isocyanate**)
 IT Polymerization
 (oligomerization, of chlorine **isocyanate**)
 IT 24604-62-4P 27341-09-9P
 (preparation of)

L50 ANSWER 43 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1970:31905 HCAPLUS
 DOCUMENT NUMBER: 72:31905
 TITLE: Carbofunctional organosilicon compounds. VI.
 Urethidinedione derivatives of
isocyanates
 AUTHOR(S): Smetankina, N. P.; Miryan, N. I.; Didkovskii,
 V. E.
 CORPORATE SOURCE: Inst. Khim. Vysokomol. Soedin., Kiev, USSR
 SOURCE: Zhurnal Obshchei Khimii (1969), 39(9), 2016-20
 CODEN: ZOKHA4; ISSN: 0044-460X
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian

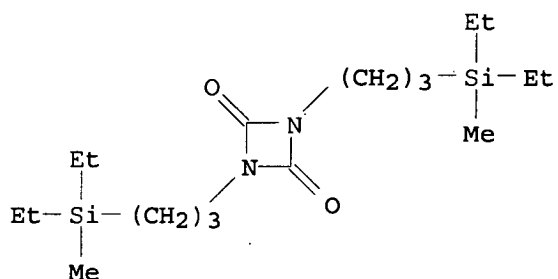
AB **Heating** 14 g Cl(CH₂)₃SiEt₃ (I) with 11.8 g KO-CN in dry
 Me₂NCHO with 0.12 g Et₄NI 10 min at 145° under argon gave
 37% Et₃Si(CH₂)₃NCO and 41.6% its dimer, b₁ 167-70°, n_D20
 1.4875. Similarly were prepared the dimers [R₃Si(CH₂)_nNCO]₂ in
 25-50% yields (R₃ and n shown); Me₃, 1, b₅ 153°, Et₃, 1,
 b₀·06 172-4°, 1.48 80; Me₃, 3, b₀·015
 120°, 14610; Ph₃, 3, b₀·04 160-2°, 1.4800;
 and MeEt₂, 3, undistd. **Heating** 2 g I with 1.6 g KO-CN
 and 0.08 g Et₄NI in Me₂NCHO 1.5 hr at 150° in argon atmospheric
 gave 70% above dimer. Ir spectral curves were shown. Thus, the
 haloalkylsilanes in reacting with KO-CN yield not only the
isocyanates but polymers with ring systems in the chain.
 The NCO group band in the **isocyanates** of Si lay in the
 2270 cm⁻¹ region, while the 1690 cm⁻¹ band is that of the CO group
 of the uretidinedione ring of the above dimers.

IT 24602-17-3P 24602-19-5P 24602-21-9P
 24602-22-0P 24602-23-1P
 (preparation of)

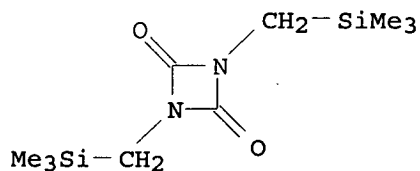
RN 24602-17-3 HCAPLUS
 CN 2,4-Urethidinedione, 1,3-bis[3-(triethylsilyl)propyl]- (8CI) (CA
 INDEX NAME)



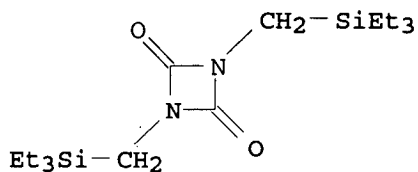
RN 24602-19-5 HCAPLUS
 CN 2,4-Uretidinedione, 1,3-bis[3-(diethylmethylsilyl)propyl]- (8CI)
 (CA INDEX NAME)



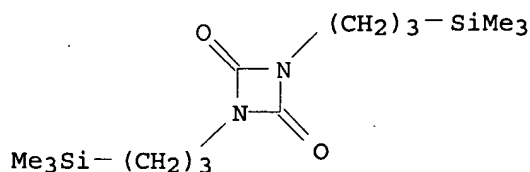
RN 24602-21-9 HCAPLUS
 CN 2,4-Uretidinedione, 1,3-bis[(trimethylsilyl)methyl]- (8CI) (CA
 INDEX NAME)



RN 24602-22-0 HCAPLUS
 CN 2,4-Uretidinedione, 1,3-bis[(triethylsilyl)methyl]- (8CI) (CA
 INDEX NAME)



RN 24602-23-1 HCAPLUS
 CN 2,4-Uretidinedione, 1,3-bis[3-(trimethylsilyl)propyl]- (8CI) (CA
 INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)
 ST silyl **isocyanate** dimers; **isocyanate** dimers
 silyl; dimers silyl **isocyanate**; urethidinediones silyl
 IT 7440-21-3DP, Silicon, organic carbonyl derivs. **24602-17-3P**
24602-18-4P 24602-19-5P 24602-20-8P
24602-21-9P 24602-22-0P 24602-23-1P
 26246-60-6P
 (preparation of)

L50 ANSWER 44 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1969:481328 HCAPLUS
 DOCUMENT NUMBER: 71:81328
 TITLE: Uretidinediones with aliphatic substituents
 PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
 SOURCE: Fr., 6 pp.
 CODEN: FRXXAK
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

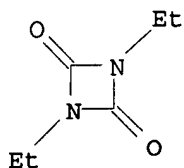
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1532054		19680705	FR	
DE 1670720			DE	
GB 1153815			GB	
PRIORITY APPLN. INFO.:			DE	
				1966
				0721

GI For diagram(s), see printed CA Issue.
 AB Substituted uretidinediones (I) are prepared by the dimerization at 60-140° of aliphatic **isocyanates** in the presence of a tertiary phosphine having ≥ 1 aliphatic substituent or BF_3 catalyst in an organic solvent and interrupting the reaction after 5-50% conversion, isolating I, and returning unreacted **isocyanates** to the reaction mixture. Thus, 657 parts freshly distilled BuNCO was heated at 60° with 9.85 parts Bu_3P for 4 hrs. or until a NCO content of 35.6% was obtained, the reaction stopped by adding 6.3 g. Me_2SO_4 , and the mixture heated at 80° to give 16.5% conversion, and the mixture fractionated at 1.2 mm. to give 546 parts BuNCO in the cold trap and forecut (b. 45-92°) 3.6, I (R = Bu) (b. 92-3°) 49.0, intermediate fraction (b. 94-154°) 1.9, isocyanurate (b. 155-8°) 40.7, and residue 13.0 parts. Similarly prepared were the following I (R and b.p./mm. given): Et, 73-4°/760, allyl, 66°/1.0; MeOCH_2 , 86°/1.0; 6-chlorohexyl, -; 5-(**isocyanatomethyl**)-3,3,5-trimethylcyclohexylmethyl, -. 1,6-Hexamethylene **diisocyanate** uretidinedione was also prepared

IT 23336-34-7P 23336-35-8P 23336-44-9P
 23336-45-0P 23336-46-1P 23501-81-7P
 (preparation of)

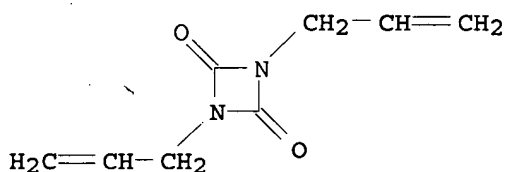
RN 23336-34-7 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-diethyl- (9CI) (CA INDEX NAME)



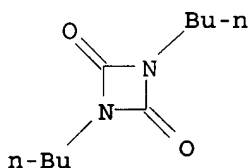
RN 23336-35-8 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-di-2-propenyl- (9CI) (CA INDEX NAME)



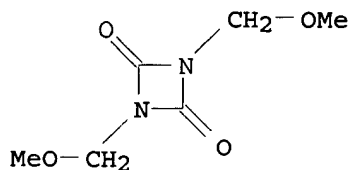
RN 23336-44-9 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-dibutyl- (9CI) (CA INDEX NAME)



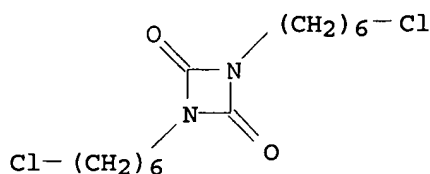
RN 23336-45-0 HCAPLUS

CN 2,4-Uretidinedione, 1,3-bis(methoxymethyl)- (8CI) (CA INDEX NAME)

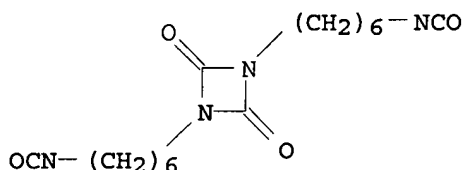


RN 23336-46-1 HCAPLUS

CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-chlorohexyl)- (9CI) (CA INDEX NAME)



RN 23501-81-7 HCAPLUS
 CN 1,3-Diazetidine-2,4-dione, 1,3-bis(6-isocyanatohexyl)- (9CI) (CA
 INDEX NAME)



IC C07D
 CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
 ST **isocyanates** dimerization; dimerization
isocyanates; uretidinediones from **isocyanates**
 IT 715-63-9P 846-74-2P 1025-15-6P 17576-39-5P 21132-72-9P
 23336-34-7P 23336-35-8P 23336-44-9P
 23336-45-0P 23336-46-1P 23370-68-5P
 23501-78-2P, s-Triazine-2,4,6(1H,3H,5H)-trione,
 1,3,5-tris(methoxymethyl)- 23501-81-7P 23544-79-8P
 (preparation of)

L50 ANSWER 45 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:75614 HCAPLUS

DOCUMENT NUMBER: 66:75614

TITLE: Preparation and properties of
 chlorofluoromethylsulfenyl pseudohalides

AUTHOR(S): Haas, Alois; Oh, Dong-Young

CORPORATE SOURCE: Univ. Goettingen, Goettingen, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1967), 100(2), 480-91

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

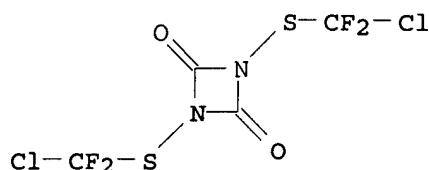
LANGUAGE: German

OTHER SOURCE(S): CASREACT 66:75614

AB Cl₂FCSCl (I) and ClF₂CSCl (II) without solvent gave with AgOCN the corresponding monomeric **isocyanates** but in C₆H₆ the isocyanurates were formed. The hydrolysis and alcoholysis of the **isocyanates** is described. ClF₂CSNCO dimerized slowly at 20° to the corresponding uretidinedione. I and II with AgSCN yielded Cl₂FCSSCN and ClF₂CSSCN, resp., which decomposed readily to (Cl₂FCS)₂ and (ClF₂CS)₂, resp., and (SCN)_x. The ir and 19F N.M.R. spectra of the new compds. are discussed. Gradual differences in the phys. and chemical properties were observed in the course of the reaction and in the behavior of the compds. with increasing degree of fluorination. Characteristic ir bands were assigned to the groups Cl₂FCS and ClF₂CS; these bands and the 19F chemical shifts can be used for the identification.

IT 14674-07-8P
 (preparation of)

RN 14674-07-8 HCAPLUS
 CN 2,4-Uretidinedione, 1,3-bis[(chlorodifluoromethyl)thio]- (8CI)
 (CA INDEX NAME)



CC 23 (Aliphatic Compounds)
 ST NMR SULFENYL PSEUDOHALIDES; CHLOROFLUOROMETHYLSULFENYL
 PSEUDOHALIDES; IR SULFENYL PSEUDOHALIDES; SULFENYL PSEUDOHALIDES;
 PSEUDOHALIDES CHLOROFLUOROMETHYLSULFENYL; **ISOCYANATES**;
 ISOCYANURATES; URETIDINEDIONES
 IT 692-58-0P 14673-88-2P 14673-90-6P 14673-91-7P 14673-92-8P
 14673-93-9P 14674-05-6P 14674-06-7P **14674-07-8P**
 14674-08-9P 14999-95-2P 15085-84-4P
 (preparation of)

L50 ANSWER 46 OF 46 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:18702 HCAPLUS

DOCUMENT NUMBER: 66:18702

TITLE: Thioacyl **isocyanates**. V.
 Substituted thiazoline-4,5-diones and their
 thermal cleavage into **isocyanates**
 and mustard oils

AUTHOR(S): Goerdeler, Joachim; Jonas, Klaus

CORPORATE SOURCE: Univ. Bonn, Bonn, Germany

SOURCE: Chemische Berichte (1966), 99(11), 3572-81
 CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 66:18702

GI For diagram(s), see printed CA Issue.

AB cf. CA 64, 19456d. A series of 2-X substituted
 4,5-dihydro-4,5-dioxothiazoles (I) with functional groups in the
 2-position was prepared and converted thermally into the
 corresponding XC(:S)NCO (II). The II were either isolated as such
 or captured with amines or PhCH:NPh. The dimerization of the II
 gave 6-(X substituted)-3-[C(:S)X substituted] 2,3-dihydro-4H-1,3,5-
 thiadiazine-2,4-diones (III) and in 1 case the
 N,N'-bis(-thionopyruvoyl)analog (IV) of diazetidinedione. All
isocyanates rearranged thermally to the corresponding
 XC(O)NCS; the rate of the rearrangement showed clearly substituent
 dependence. Me₂NCSNH₂ (1 g.) and 3.3 cc. Et₃N in 150 cc. AcOEt
 and 1 cc. (COCl)₂ in 30 cc. AcOEt added simultaneously dropwise
 with stirring at -30° to 100 cc. dry AcOEt and warmed to
 4° yielded 0.8 g. yellow I (X = Me₂N), m. 190°
 (decomposition) (repptd. from dry CHCl₃ with petroleum ether).
 Similarly were prepared the following I (X, m.p. with decomposition, and
 % yield given): Et₂N, 90° (repptd. from C₆H₆ with petroleum
 ether), 71; piperidino (V), 126° (AcOEt), 73; MePhN,
 140° (repptd. from CHCl₃ with petroleum ether), 73; EtPhN
 (VI), 160° (repptd. from CHCl₃ with petroleum ether), 75;
 BuPhN, 118° (petroleum ether-AcOEt), 65. The appropriate
 O-alkyl or aryl thiocarbamate in CH₂Cl₂ and an equivalent amount (COCl)₂

in CH₂Cl₂ added dropwise simultaneously at 0° dropwise during about 0.5 hr. to dry CH₂Cl₂ or (CH₂Cl)₂ and evaporated rapidly yielded the corresponding I. In this manner were prepared the following I (X, m.p., and % yield given): MeO, 118° (decomposition) (repptd. from C₆H₆ with petroleum ether), 69; EtO, 44-6° (petroleum ether), 65; PhO (VII), 118-20° (decomposition), 72; cyclohexyloxy (VIII), 97° (decomposition) (repptd. from C₆H₆ with petroleum ether), 52. H₂NCS₂Me (1.1 g.) in 20 cc. CH₂Cl₂ and 1 cc. (COCl)₂ in 20 cc. CH₂Cl₂ added to 30 cc. CH₂Cl₂ at 0° gave 1.2 g. canary-yellow I (X = MeS) (IX), m. 108° (decomposition). O-Cyclohexyl thiocarbamate (1.6 g.) in 15 cc. CH₂Cl₂ and 1 cc. (COCl)₂ in 15 cc. CH₂Cl₂ added dropwise simultaneously at 0° to 15 cc. CH₂Cl₂ gave 1.1 g. thiazolidine-2,4,5-trione, m. 158°. The appropriate I and stainless steel spirals distilled in vacuo into a receiver cooled at -60° gave the corresponding II (X, m.p., nD/temp., temperature, and pressure in mm. Hg given): MeO (X), -, 1.498/24°, 63, 120°, 120; EtO (XI), -, 1.492/19°, 67, 110°, 14; PhO, -24 to -22°, 1.500/20°, 86, 135°, 0.4; cyclohexyloxy, about 30°, 1.520/16°, 77, 120°, 0.4; MeS, -22 to -20°, -, 78, 120°, 14. XI kept 3 days at -20° in a little C₆H₆, diluted with petroleum ether, and cooled to -30° gave nearly quant. III (X = EtO), m. 80° (decomposition). Similarly were prepared the following III in nearly quant. yields (X, m.p., reaction temperature, and reaction time given): cyclohexyloxy, 90-100° (decomposition), room temperature, 30 hrs.; PhO, about 140°, room temperature, 15 min.; MeS, 142° (decomposition), -20°, overnight. Crystalline V (1 g.) kept 3 min. at 140° in vacuo and cooled to 0° gave 0.4 g. III (X = piperidino) (XII), m. 160° (decomposition). X kept 20 hrs. at -60 to -20° and the product repptd. from AcOEt with petroleum ether at 0° gave nearly 100% IV, m. 170° (decomposition). The appropriate I (2.5 millimoles) and 0.45 g. PhCH:NPh in 10 cc. MePh heated 4 min. at 100° gave the corresponding 2,3,5,6-tetrahydro-4H-2-(X-substituted)-6-phenyl-1,3,5-thiadiazin-4-ones (XIII) (X, m.p. with decomposition, and % yield given): EtPhN, 170-5°, 93; MeO, 160°, 94; PhO, 140-50°, 95; cyclohexyloxy, 180-90°, 76; Ph₂N, 170-5°, 90. XII (0.4 g.) and 0.35 g. p-O₂NC₆H₄NH₂ in 40 cc. MePh kept 5 hrs. at 60° yielded 0.4 g. beige XC(:S)NHCONHAr (XIV) (X = piperidino, Ar = p-O₂NC₆H₄), m. 204° (decomposition). 2-Diphenyl laminothiazoline-4,5-dione (0.35 g.) in 10 cc. MePh heated 3 min. at 100°, cooled to 0°, treated with 0.15 g. PhNH₂, and kept 1 hr. at room temperature gave 0.25 g. XIV (X = Ph₂N, Ar = Ph), m. 135-7° (decomposition) (petroleum ether). I (X = MeO) (0.35 g.) and 0.25 g. PhNH₂ gave similarly 0.5 g. XIV (X = MeO, Ar = Ph). VII (0.5 g.) and 0.25 g. PhNH₂ gave similarly during 0.5 hr. at room temperature 0.65 g. XIV (X = PhO, Ar = Ph), m. 182-4° (decomposition) (ligroine, b. 100-40°). VIII (0.5 g.) in 15 cc. MePh kept 4 min. at 100°, cooled to 0°, and treated with 2.5 g. PhNH₂ gave 0.6 g. XIV (X = cyclohexyloxy, Ar = Ph), m. 136° (ligroine). II (X = MeS) (1.3 g.) and 0.9 g. PhNH₂ gave similarly 2.15 g. XIV (X = MeS, Ar = Ph), m. 200-5° (decomposition) (ligroine). V (0.5 g.) in 100 cc. MePh kept 20 min. at 100°, cooled to room temp., and treated 1 hr. with 0.25 g. PhNH₂ yielded 0.6 g. N-piperidinoformyl-N'-phenylthiourea (XV), m. 125° (decomposition) (ligroine). V (0.5 g.) and 0.35 g. p-O₂NC₆H₄NH₂ gave

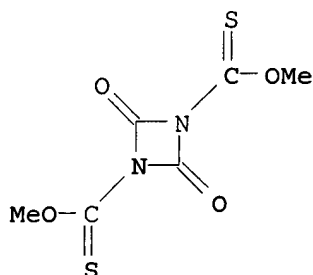
similarly at room temperature during 2 hrs. 0.6 g. beige p-NO₂ derivative of XV, m. 152° (decomposition) (EtOH). VI (0.6 g.) with 0.35 g. p-O₂NC₆H₄NH₂ gave similarly 0.7 g. p-O₂NC₆H₄NHCSNHO₂CNEtPh, m. 180° (decomposition) (Me₂CO). IX (0.4 g.) and 0.25 g. PhNH₂ yielded 0.45 g. MeSCONHCSNHPh, m. 168° (decomposition) (petroleum ether-AcOEt).

IT 13163-42-3P

(preparation of)

RN 13163-42-3 HCAPLUS

CN 1,3-Uretidinedicarbothioic acid, 2,4-dioxo-, O,O'-dimethyl ester (8CI) (CA INDEX NAME)



CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

ST **ISOCYANATES** THIOACYL; THIAZOLINEDIONES; MUSTARD OILS;
THIOACYL **ISOCYANATES**; THIAZOLINEDIONES;
ISOCYANATES THIOACYL; THIOACYL **ISOCYANATES**;
MUSTARD OILS

IT Allophanic acid, 4-phenyl-1,3-dithio-, S-methyl ester

Biuret, 1,1,5-triphenyl-2-thio-

Carbonic acid, dithio-, monoanhydride with isocyanic acid,
s-methyl ester

Carbonic acid, dithio-, monoanhydride with isocyanic acid,
s-methyl ester

Formic acid, **isocyanatodithio**-, methyl ester
(preparation of)

IT 5729-32-8P 13163-09-2P 13163-10-5P 13163-11-6P 13163-12-7P

13163-13-8P 13163-20-7P 13163-31-0P 13163-32-1P

13163-33-2P 13163-34-3P 13163-35-4P 13163-36-5P, Isocyanic
acid, anhydride with s-methyl dithiocarbonate 13163-36-5P

13163-37-6P 13163-38-7P 13163-39-8P 13163-40-1P

13163-41-2P **13163-42-3P** 13163-43-4P 13163-44-5P

13163-45-6P 13163-46-7P 13163-47-8P 13163-49-0P

13163-50-3P 13163-51-4P 13163-52-5P 13163-53-6P

13163-54-7P 13332-83-7P 13332-84-8P 13332-85-9P

13332-86-0P 13332-87-1P 13559-72-3P

(preparation of)